

FILECOPY

10/721,015

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(FILE 'HOME' ENTERED AT 17:46:02 ON 18 JAN 2006)

FILE 'REGISTRY' ENTERED AT 17:46:16 ON 18 JAN 2006 .

L1 STR  
L2 3144 SEA SSS FUL L1  
L3 STR  
L4 207 SEA SUB=L2 SSS FUL L3  
L15 STR  
L17 2 SEA SUB=L4 SSS FUL L15

FILE 'HCAPLUS' ENTERED AT 18:17:14 ON 18 JAN 2006

L18 1 SEA ABB=ON PLU=ON L17  
D STAT QUE L18  
D IBIB ABS HITSTR L18 1

FILE 'REGISTRY' ENTERED AT 18:17:52 ON 18 JAN 2006

L19 205 SEA ABB=ON PLU=ON L4 NOT L17

FILE 'HCAPLUS' ENTERED AT 18:18:03 ON 18 JAN 2006

L20 15 SEA ABB=ON PLU=ON L19  
L21 14 SEA ABB=ON PLU=ON L20 NOT L18  
D STAT QUE L21  
D IBIB ABS HITSTR L21 1-14  
L22 24 SEA ABB=ON PLU=ON "TONG LING"/AU  
L23 23 SEA ABB=ON PLU=ON L22 NOT (L18 OR L21)  
D STAT QUE L23 NOS  
D IBIB ABS L23 1-23  
L24 30 SEA ABB=ON PLU=ON (("SHANKAR B"/AU OR "SHANKAR B B"/AU) OR  
("SHANKAR BANDARPALLE"/AU OR "SHANKAR BANDARPALLE B"/AU OR  
"SHANKAR BANDERPALLE B"/AU)) NOT (L18 OR L21 OR L23)  
D STAT QUE L24  
D IBIB ABS L24 1-30  
L25 104 SEA ABB=ON PLU=ON (("KOZLOWSKI J"/AU OR "KOZLOWSKI J A"/AU)  
OR ("KOZLOWSKI JOSEPH"/AU OR "KOZLOWSKI JOSEPH A"/AU OR  
"KOZLOWSKI JOSEPH ANDREW"/AU)) NOT (L18 OR L21 OR L23 OR L24)  
L26 105 SEA ABB=ON PLU=ON ("SHIH N"/AU OR "SHIH N Y"/AU OR ("SHIH  
NENG Y"/AU OR "SHIH NENG YANG"/AU)) NOT (L18 OR L21 OR L23 OR  
L24)  
L27 2852 SEA ABB=ON PLU=ON ("CHEN L"/AU OR "CHEN L A"/AU OR "CHEN L  
ALEX"/AU OR "CHEN L B"/AU OR "CHEN L BO"/AU OR "CHEN L C"/AU  
OR "CHEN L C L"/AU OR "CHEN L C M"/AU OR "CHEN L CHARLIE"/AU  
OR "CHEN L CHUN"/AU OR "CHEN L D"/AU OR "CHEN L E"/AU OR "CHEN  
L F"/AU OR "CHEN L F O"/AU OR "CHEN L G"/AU OR "CHEN L H"/AU  
OR "CHEN L H K"/AU OR "CHEN L I"/AU OR "CHEN L J"/AU OR "CHEN  
L JENNY"/AU OR "CHEN L K"/AU OR "CHEN L L"/AU OR "CHEN L M"/AU  
OR "CHEN L MICHAEL"/AU OR "CHEN L N"/AU OR "CHEN L P"/AU OR  
"CHEN L Q"/AU OR "CHEN L R"/AU OR "CHEN L S"/AU OR "CHEN L  
T"/AU OR "CHEN L W"/AU OR "CHEN L W A"/AU OR "CHEN L W  
ANTONY"/AU OR "CHEN L X"/AU OR "CHEN L X Q"/AU OR "CHEN L  
Y"/AU OR "CHEN L Z"/AU OR "CHEN L ZHONG"/AU) OR CHEN LEI ?/AU  
L28 0 SEA ABB=ON PLU=ON L25 AND L26 AND L27  
L29 5 SEA ABB=ON PLU=ON L25 AND (L26 OR L27)  
L30 0 SEA ABB=ON PLU=ON L26 AND L27  
L31 2 SEA ABB=ON PLU=ON (L25 OR L26 OR L27) AND CANNABI?  
L32 45 SEA ABB=ON PLU=ON (L25 OR L26 OR L27) AND LIGAND  
L33 50 SEA ABB=ON PLU=ON L28 OR L29 OR L30 OR L31 OR L32  
D STAT QUE L33  
D IBIB ABS L33 1-50

## FILE HOME

## FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 JAN 2006 HIGHEST RN 872085-61-5  
 DICTIONARY FILE UPDATES: 17 JAN 2006 HIGHEST RN 872085-61-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****~*****
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Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

## FILE HCAPLUS

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FILE COVERS 1907 - 18 Jan 2006 VOL 144 ISS 4  
 FILE LAST UPDATED: 17 Jan 2006 (20060117/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> fil hcaplus  
 FILE 'HCAPLUS' ENTERED AT 18:17:14 ON 18 JAN 2006  
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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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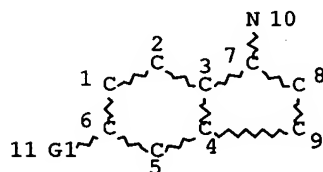
FILE COVERS 1907 - 18 Jan 2006 VOL 144 ISS 4  
 FILE LAST UPDATED: 17 Jan 2006 (20060117/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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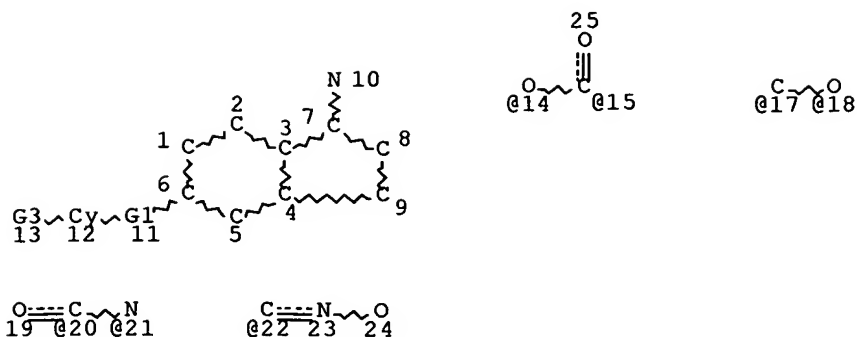
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 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE  
 L2 3144 SEA FILE=REGISTRY SSS FUL L1  
 L3 STR



VAR G1=C/S/O/N/14-6 15-12/15-6 14-12/17-6 18-12/20-6 21-12/21-6 20-12/22

VAR G3=AK/CY/C/S/O/N

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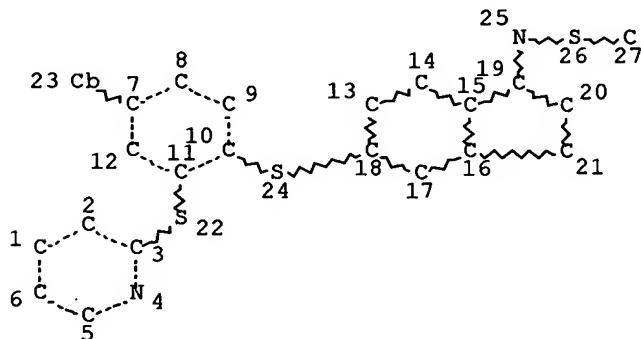
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L4 207 SEA FILE=REGISTRY SUB=L2 SSS FUL L3

L15 STR ,



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L17 2 SEA FILE=REGISTRY SUB=L4 SSS FUL L15

L18 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L17

=>

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=&gt; d ibib abs hitstr l18 1

L18 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:467852 HCAPLUS Full-text

DOCUMENT NUMBER: 141:38447

TITLE: Preparation of indanesulfonamides and related compounds as cannabinoid CB2 receptor ligands

INVENTOR(S): Tong, Ling; Chen, Lei; Shankar, Bandarpalle B.; Kozlowski, Joseph A.; Shih, Neng-Yang

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 71 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

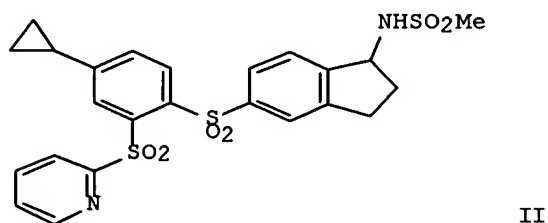
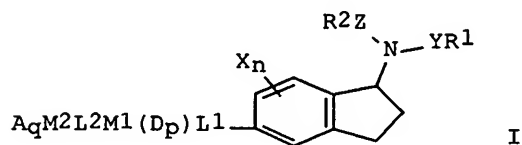
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004048322	A1	20040610	WO 2003-US37366	20031121
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2506895	AA	20040610	CA 2003-2506895	20031121
US 2004132804	A1	20040708	US 2003-721015	20031121
EP 1565431	A1	20050824	EP 2003-789933	20031121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			US 2002-428861P	P 20021125
			WO 2003-US37366	W 20031121

OTHER SOURCE(S): MARPAT 141:38447

GI



AB Title compds. [I; R1, R2 = H, CF3, (substituted) alkyl, alkoxy, cycloalkyl, heterocycloalkyl, heteroaryl, etc.; R1YNZR2 = atoms to form a 4-8 membered (substituted) heterocycloalkyl; X = alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; L1 = C(R2)2, O2C, CO, S, SO2, SO, NHCO, etc.; L2 = bond, C(R2)2, S, SO, SO2, O, N(R2)2, CONH, CF2, etc.; M1 = (substituted) aryl, heteroaryl, cycloalkyl, heterocycloalkyl; M2 = (substituted) alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl; n = 0-3; p = 0-4; q = 0-5], were prepared. Thus, title compound (II) (multistep preparation from 5-bromo-1-indanone given) showed CB2 inhibitory activity with  $K_i < 20$  nM.

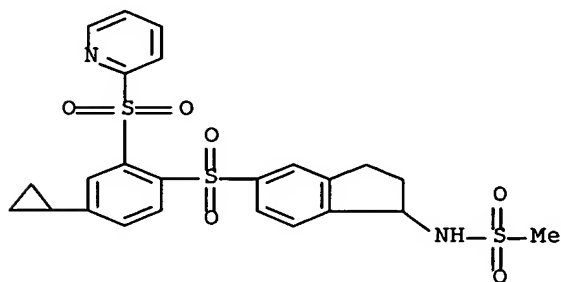
IT 701268-02-2P 701268-09-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of indanesulfonamides and related compds. as cannabinoid CB2 receptor ligands)

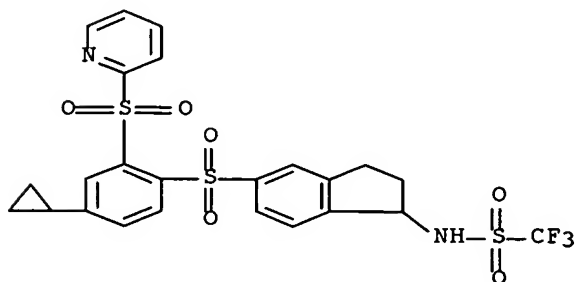
RN 701268-02-2 HCAPLUS

CN Methanesulfonamide, N-[5-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-2,3-dihydro-1H-inden-1-yl]- (9CI) (CA INDEX NAME)



RN 701268-09-9 HCAPLUS

CN Methanesulfonamide, N-[5-[[4-cyclopropyl-2-(2-pyridinylsulfonyl)phenyl]sulfonyl]-2,3-dihydro-1H-inden-1-yl]-1,1,1-trifluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

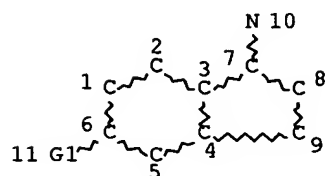
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THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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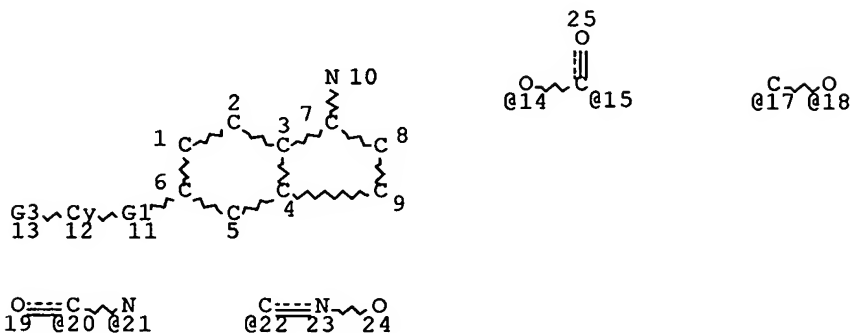
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VAR G1=C/S/O/N  
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NUMBER OF NODES IS 11

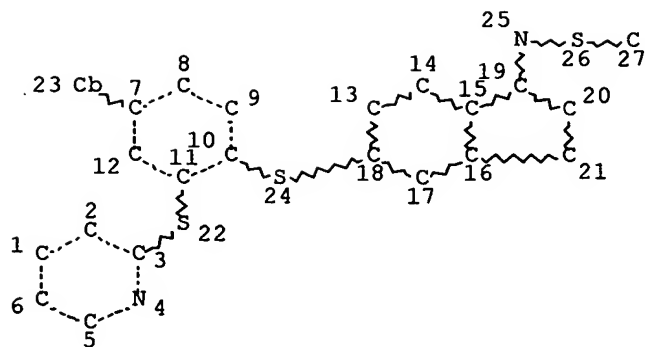
STEREO ATTRIBUTES: NONE  
L2 3144 SEA FILE=REGISTRY SSS FUL L1  
L3 STR



VAR G1=C/S/O/N/14-6 15-12/15-6 14-12/17-6 18-12/20-6 21-12/21-6 20-12/22  
VAR G3=AK/CY/C/S/O/N  
NODE ATTRIBUTES:  
NSPEC IS RC AT 10  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
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NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE  
L4 207 SEA FILE=REGISTRY SUB=L2 SSS FUL L3  
L15 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L17 2 SEA FILE=REGISTRY SUB=L4 SSS FUL L15  
 L18 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L17  
 L19 205 SEA FILE=REGISTRY ABB=ON PLU=ON L4 NOT L17  
 L20 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L19  
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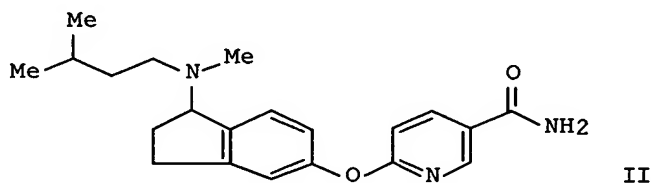
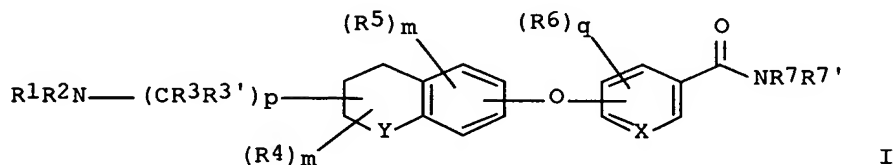
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=> d ibib abs hitstr l21 1-14

L21 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:780668 HCAPLUS Full-text  
 DOCUMENT NUMBER: 141:295866  
 TITLE: Preparation of 6-substituted nicotinamides as opioid  
 receptor antagonists for treating obesity and related  
 diseases  
 INVENTOR(S): Pedregal-Tercero, Concepcion; Siegel, Miles Goodman;  
 Stucky, Russell Dean; Takeuchi, Kumiko  
 PATENT ASSIGNEE(S): Eli Lilly and Company, USA  
 SOURCE: PCT Int. Appl., 129 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004080968	A1	20040923	WO 2004-US3360	20040225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,				

TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,  
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,  
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,  
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 CA 2518194 AA 20040923 CA 2004-2518194 20040225  
 EP 1613597 A1 20060111 EP 2004-714542 20040225  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 PRIORITY APPLN. INFO.: US 2003-453414P P 20030307  
 WO 2004-US3360 W 20040225  
 OTHER SOURCE(S): MARPAT 141:295866  
 GI



AB Title compds. I [wherein X = C, N; p, y, z = independently 0-3; n = 0-2; R1, R2 = independently H, (un)substituted alk(en/yn)yl, alkylaryl, alkoxyalkyl, etc.; or R1NR2 = (un)substituted 4- to 7-member nitrogen-containing heterocycle; R3, R3' = independently H, alk(en/yn)yl, Ph, alkyl/aryl; each R4, R5, R6 = independently alk(en/yn)yl, alkoxy, halo, haloalkyl, Ph, alkyl/aryl, C(:O)-alkyl, etc.; each R7, R7' = independently H, OH and derivs., (un)substituted alk(en/yn)yl, alkyl/aryl, SO2-alkylheterocyclyl, etc.; or R7NR7' = (un)substituted 4- to 7-member nitrogen-containing heterocycle; and their pharmaceutically acceptable salts, enantiomers, racemates, diastereomers or solvates] were prepared as  $\mu$ -,  $\kappa$ -, and  $\delta$ -opioid receptor antagonists. For example, II was prepared by reacting 6-[(4-methyl-1-oxoindan-5-yl)oxy]nicotinamide (preparation given) with N-methylisoamylamine in the presence of Ti(i-OPr)<sub>4</sub> in THF. In the [35S]GTP- $\gamma$ -S binding assay, II bound to  $\mu$ -,  $\kappa$ -, and  $\delta$ -opioid receptor with a K<sub>b</sub> of 0.73, 2.5, and 13.48, resp. Thus, I and their formulations are useful for treating obesity and related disorders.

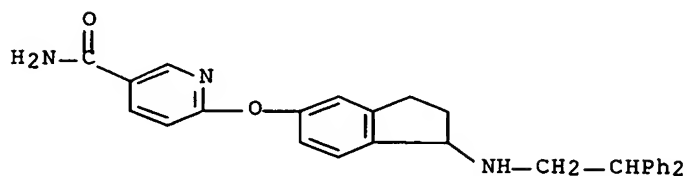
IT **762173-17-1P**, 6-[1-(2,2-Diphenylethylamino)indan-5-yl]oxy]nicotinamide **762173-20-6P**, 6-(1-Hexylaminoindan-5-yloxy)nicotinamide **762173-26-2P**, 6-[1-[2-(Phenyl)ethylamino]indan-5-yloxy]nicotinamide

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(opioid receptor antagonist; preparation of nicotinamides as opioid receptor antagonists for treating obesity and related diseases)

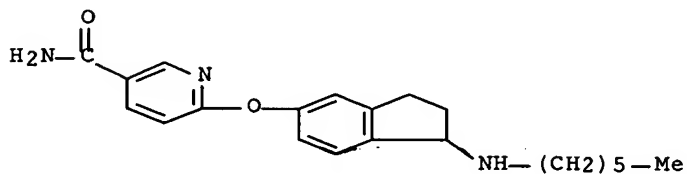
RN 762173-17-1 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[(2,2-diphenylethyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



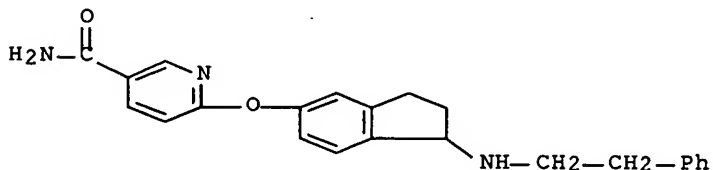
RN 762173-20-6 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-(hexylamino)-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762173-26-2 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(2-phenylethyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



IT 762173-09-1P, 6-[[1-(3-Methylbutylamino)indan-5-yl]oxy]nicotinamide 762173-10-4P, 6-[[1-[[2-(Thiophen-2-yl)ethyl]amino]indan-5-yl]oxy]nicotinamide 762173-11-5P, 6-[[1-[[2-(4-Methoxybenzo[b]thiophen-3-yl)ethyl]amino]indan-5-yl]oxy]nicotinamide 762173-13-7P, 6-[[1-[[2-(3-Chlorophenyl)ethyl]amino]indan-5-yl]oxy]nicotinamide 762173-15-9P, 6-[[1-[[2-(2-Fluorophenyl)ethyl]amino]indan-5-yl]oxy]nicotinamide 762173-19-3P, 6-[[1-(3-Phenylpropylamino)indan-5-yl]oxy]nicotinamide 762173-21-7P, 6-[[1-[(2,2-Diphenylethyl)(methyl)amino]indan-5-yl]oxy]nicotinamide 762173-22-8P, 6-[[1-[[2-(m-Tolyl)ethyl]amino]indan-5-yl]oxy]nicotinamide 762173-23-9P, 6-[1-(Hexylmethylamino)indan-5-yloxy]nicotinamide 762173-24-0P, 6-[[1-(2-Cyclohexylethylamino)indan-5-yl]oxy]nicotinamide 762173-25-1P, 6-(3,3-Dimethyl-1-phenethylamino)indan-5-yloxy]nicotinamide 762173-27-3P, 6-(4-Methyl-1-[2-(phenyl)ethylamino]indan-5-yloxy]nicotinamide 762173-28-4P, 6-[[1-[Methyl(3-

methylbutyl)amino]indan-5-yl]oxy]nicotinamide **762173-29-5P**,  
 6-[[1-[(Methyl)[2-(phenyl)ethyl]amino]indan-5-yl]oxy]nicotinamide  
**762173-33-1P**, 6-(1-Pentylaminoindan-5-yloxy)nicotinamide  
**762173-47-7P**, 6-[[1-[[2-(3-Fluorophenyl)ethyl]amino]indan-5-  
 yl]oxy]nicotinamide **762173-55-7P**, 6-[[1-(4-  
 Methylcyclohexylamino)indan-5-yl]oxy]nicotinamide **762173-85-3P**,  
 6-[[1-[(2-Methylsulfanylethyl)amino]indan-5-yl]oxy]nicotinamide  
**762173-87-5P**, 6-[[1-[[2-(3-Methoxyphenyl)ethyl]amino]indan-5-  
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 , 6-[[1-[[2-(Pyrrolidin-1-yl)ethyl]amino]indan-5-yl]oxy]nicotinamide  
**762173-93-3P**, 6-[[1-[[2-(Pyridin-2-yl)ethyl]amino]indan-5-  
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**762173-98-8P**, 6-[[1-[[2-(4-Fluorophenyl)ethyl]amino]indan-5-  
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 6-[[1-[[2-(5-Fluoro-1H-indol-3-yl)ethyl]amino]indan-5-yl]oxy]nicotinamide  
**762174-04-9P**, 3-[[5-(5-Carbamoylpyridin-2-yloxy)indan-1-  
 yl]amino]propionic acid isopropyl ester **762174-22-1P**,  
 6-[[1-[[[Benzo[b]thiophen-3-yl)methyl]amino]indan-5-yl]oxy]nicotinamide  
**762174-24-3P**, 6-[[1-(2-Methoxyethylamino)indan-5-  
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 Trifluoromethylphenyl)ethyl]amino]indan-5-yl]oxy]nicotinamide  
**762174-29-8P**, 6-[[1-[[2-(4-Fluorophenyl)-1,1-  
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 6-[[1-(3-Hydroxypropylamino)indan-5-yl]oxy]nicotinamide  
**762174-33-4P**, 6-[[1-(2,2,2-Trifluoroethylamino)indan-5-  
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**762174-42-5P**, 6-[1-(4-Thiomorpholinyl)indan-5-yloxy]nicotinamide  
**762174-45-8P**, 6-[[1-(5-Oxo-[1,4]diazepan-1-yl)indan-5-  
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**762174-49-2P**, 6-[1-(3-Phenylpyrrolidin-1-yl)indan-5-  
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**762174-52-7P**, 6-(1-Decylaminoindan-5-yloxy)nicotinamide  
**762174-53-8P**, 6-[[1-(2-Ethylhexylamino)indan-5-yl]oxy]nicotinamide  
**762174-54-9P**, 6-[[1-[(Tetrahydrofuran-2-yl)methyl]amino]indan-5-  
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**762174-57-2P**, 6-[[1-(Cyclopropylamino)indan-5-yl]oxy]nicotinamide  
**762174-58-3P**, 6-[[1-(1,3-Dimethylbutylamino)indan-5-  
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 , 6-[[1-(Cyclobutylamino)indan-5-yl]oxy]nicotinamide **762174-62-9P**  
 , 6-[[1-(Cyclopentylamino)indan-5-yl]oxy]nicotinamide **762174-63-0P**  
 , 6-[[1-[(Cyclohexylmethyl)amino]indan-5-yl]oxy]nicotinamide  
**762174-64-1P**, 6-[[1-[(1-Ethylpyrrolidin-2-yl)methyl]amino]indan-5-  
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 (Cyclohexylamino)propyl]amino]indan-5-yl]oxy]nicotinamide **762174-66-3**  
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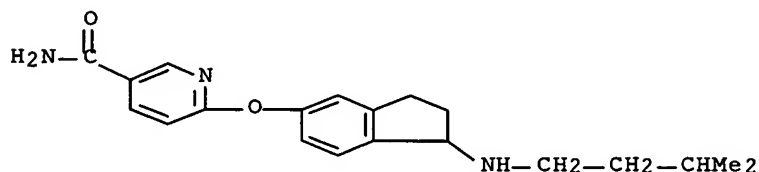
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**762174-68-5P**, 6-[[1-[(1-Isopropyl-2-methylpropyl)amino]indan-5-yl]oxy]nicotinamide **762174-69-6P**, 6-[[1-(2-Cyclohex-1-enylethylamino)indan-5-yl]oxy]nicotinamide **762174-70-9P**,  
 6-[[1-(2-Methylbutylamino)indan-5-yl]oxy]nicotinamide **762174-71-0P**  
**762174-72-1P**, 6-[[1-(1,4-Dimethylpentylamino)indan-5-yl]oxy]nicotinamide **762174-73-2P**, 6-[[1-(1-Cyclohexylethylamino)indan-5-yl]oxy]nicotinamide **762174-74-3P**,  
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**762174-75-4P**, 6-[[1-(2-Carbamoylcyclohexylamino)indan-5-yl]oxy]nicotinamide **762174-76-5P**, 6-[[1-[(Cyclopropylmethyl)amino]indan-5-yl]oxy]nicotinamide **762174-77-6P**,  
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**762174-78-7P**, 6-[[1-[(2,2,3,3,4,4,4-Heptafluorobutyl)amino]indan-5-yl]oxy]nicotinamide **762174-79-8P**, 6-[[1-[[3-(2-Oxopyrrolidin-1-yl)propyl]amino]indan-5-yl]oxy]nicotinamide **762174-80-1P**,  
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**762174-81-2P**, 6-[[1-(2,2,3,3,3-Pentafluoropropylamino)indan-5-yl]oxy]nicotinamide **762174-82-3P**, 6-[[1-[(2-Hydroxycyclooctyl)methyl]amino]indan-5-yl]oxy]nicotinamide  
**762174-83-4P** **762174-84-5P**, 6-[[1-(2-Hydroxycyclohexylamino)indan-5-yl]oxy]nicotinamide **762174-85-6P**,  
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**762174-86-7P**, 6-[[1-[[2-(4-Methylcyclohexyl)ethyl]amino]indan-5-yl]oxy]nicotinamide **762174-87-8P**, 6-[[1-(2-Cyclopentylethylamino)indan-5-yl]oxy]nicotinamide **762175-17-7P**,  
 4-[[1-[[2-(3-Fluorophenyl)ethyl]amino]indan-5-yl]oxy]benzamide  
**762175-18-8P**, 4-(1-Phenethylamino)indan-5-yloxy]benzamide  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(opioid receptor antagonist; preparation of nicotinamides as opioid receptor

antagonists for treating obesity and related diseases)

RN 762173-09-1 HCAPLUS

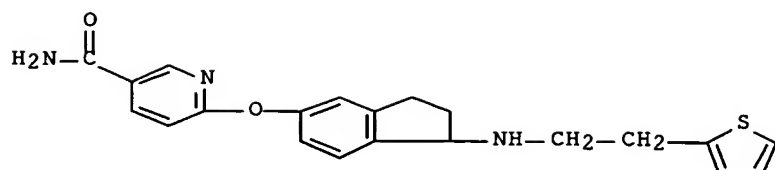
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(3-methylbutyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762173-10-4 HCAPLUS

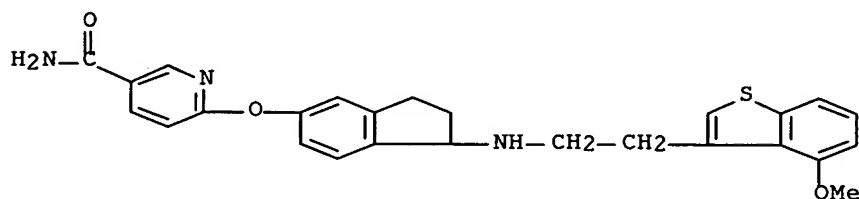
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-(2-thienyl)ethyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)





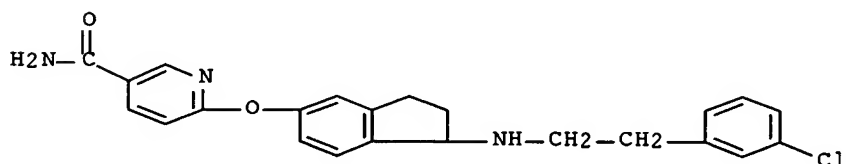
RN 762173-11-5 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-(4-methoxybenzo[b]thien-3-yl)ethyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



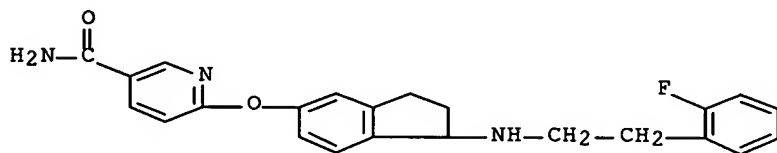
RN 762173-13-7 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[2-(3-chlorophenyl)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



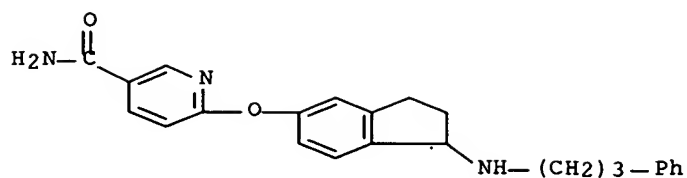
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CN 3-Pyridinecarboxamide, 6-[[1-[[2-(2-fluorophenyl)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



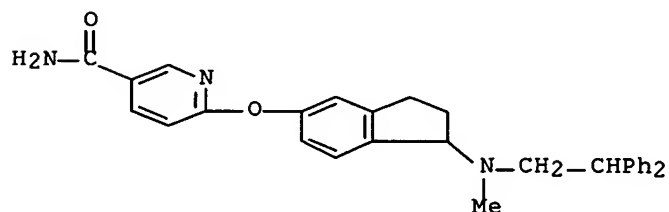
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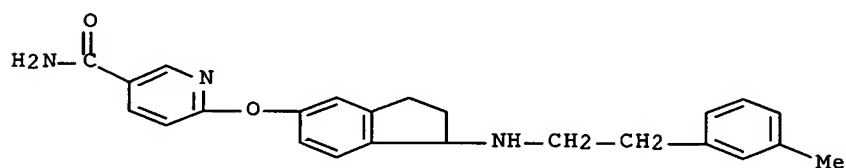
RN 762173-21-7 HCAPLUS

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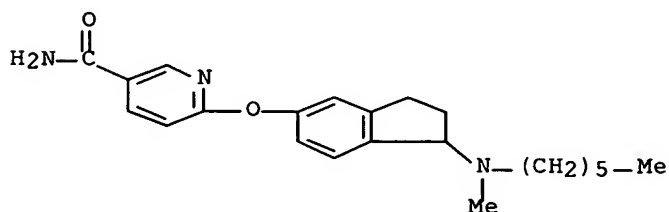
RN 762173-22-8 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-(3-methylphenyl)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



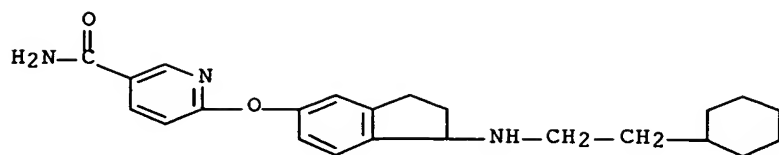
RN 762173-23-9 HCAPLUS

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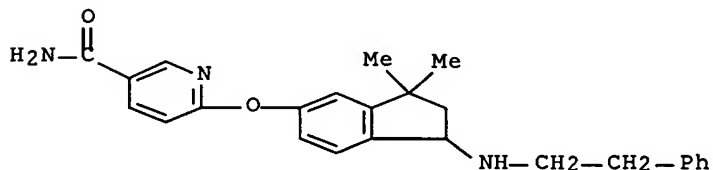
RN 762173-24-0 HCAPLUS

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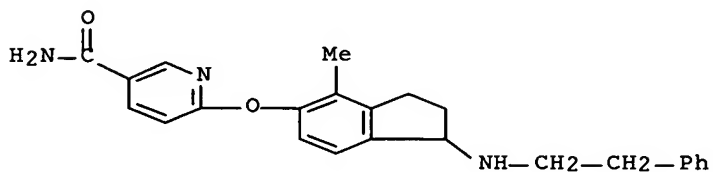
RN 762173-25-1 HCAPLUS

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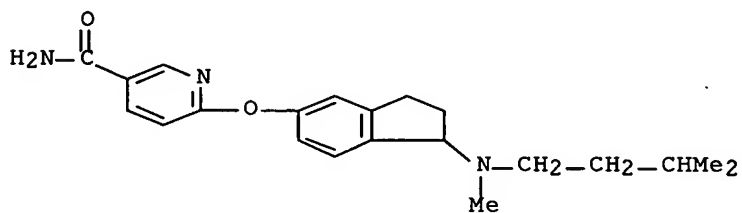
RN 762173-27-3 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-4-methyl-1-[(2-phenylethyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



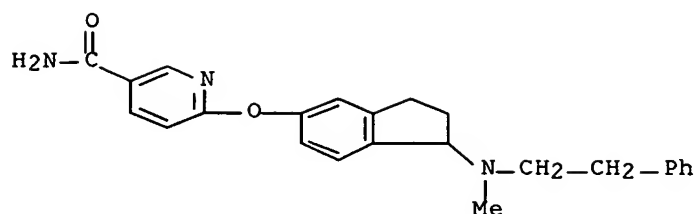
RN 762173-28-4 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[methyl(3-methylbutyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



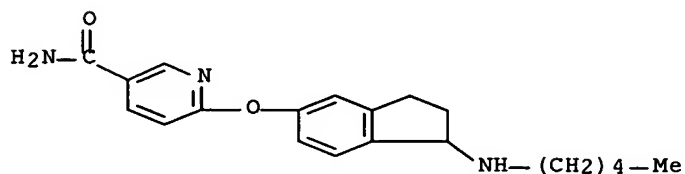
RN 762173-29-5 HCAPLUS

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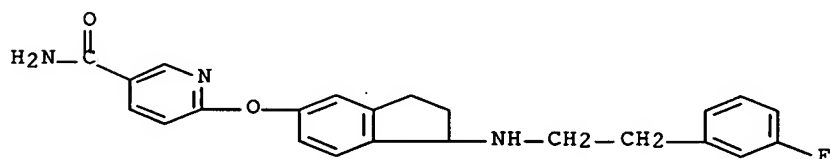
RN 762173-33-1 HCAPLUS

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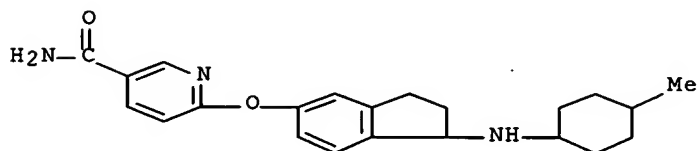
RN 762173-47-7 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[2-(3-fluorophenyl)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



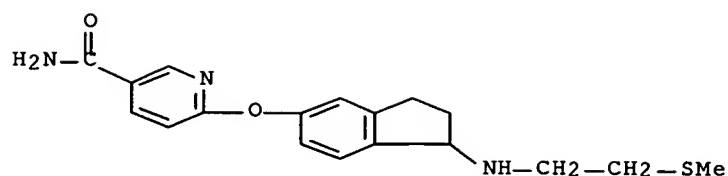
RN 762173-55-7 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(4-methylcyclohexyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



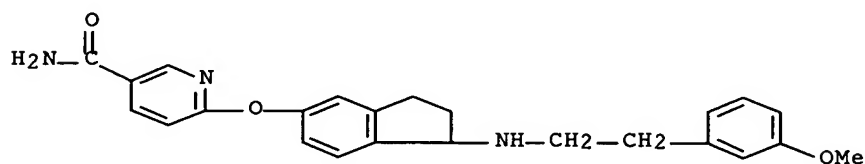
RN 762173-85-3 HCAPLUS

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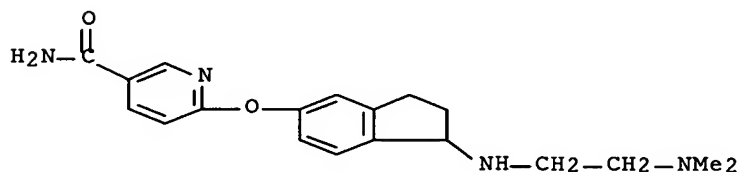
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CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-(3-methoxyphenyl)ethyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



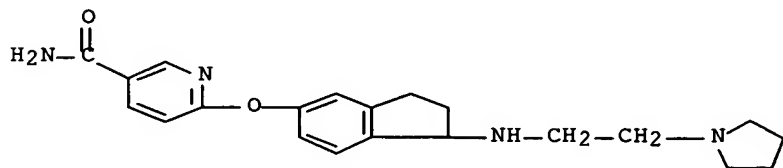
RN 762173-89-7 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[2-(dimethylamino)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



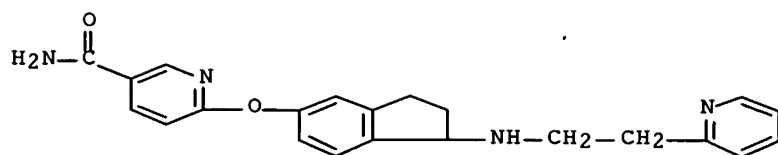
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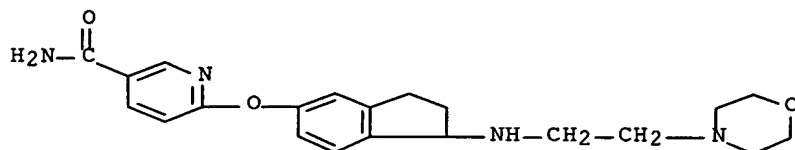
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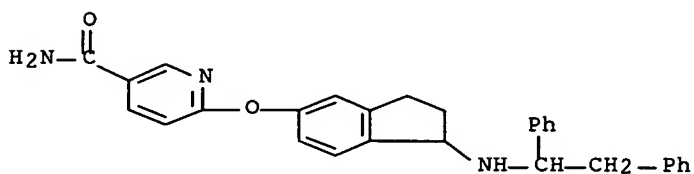
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CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-(4-morpholinyl)ethyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



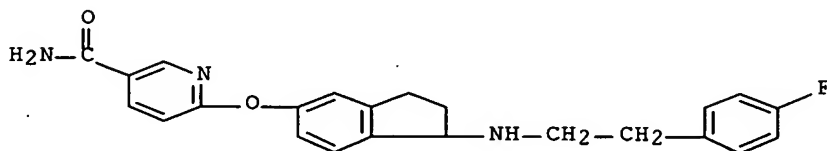
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CN 3-Pyridinecarboxamide, 6-[[1-[(1,2-diphenylethyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



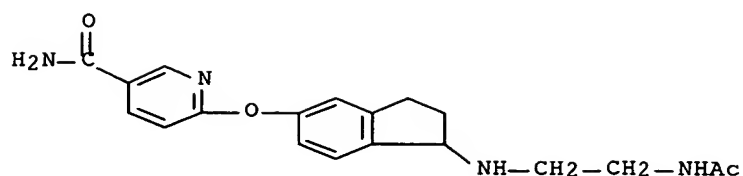
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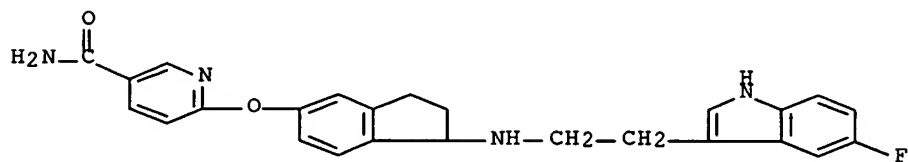
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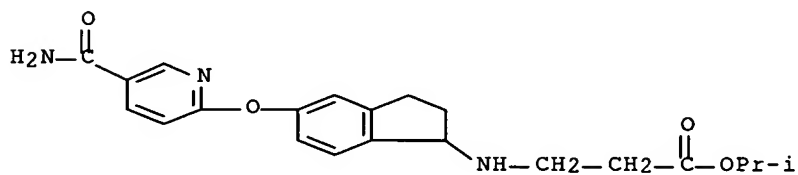
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CN 3-Pyridinecarboxamide, 6-[[1-[[2-(5-fluoro-1H-indol-3-yl)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



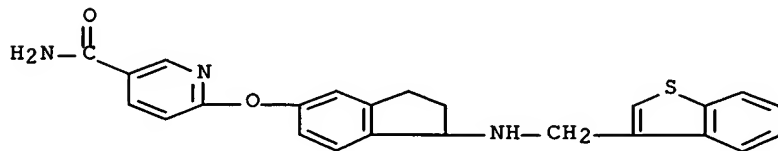
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CN  $\beta$ -Alanine, N-[5-[[5-(aminocarbonyl)-2-pyridinyl]oxy]-2,3-dihydro-1H-inden-1-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)



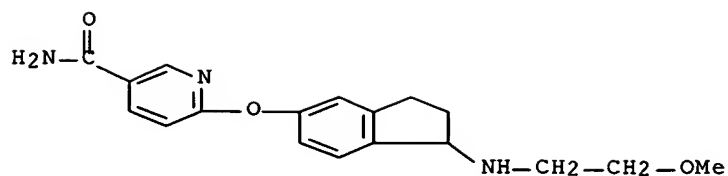
RN 762174-22-1 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[(benzo[b]thien-3-ylmethyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



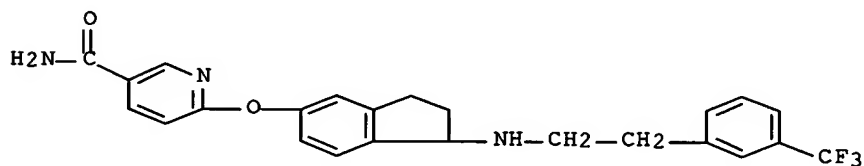
RN 762174-24-3 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(2-methoxyethyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



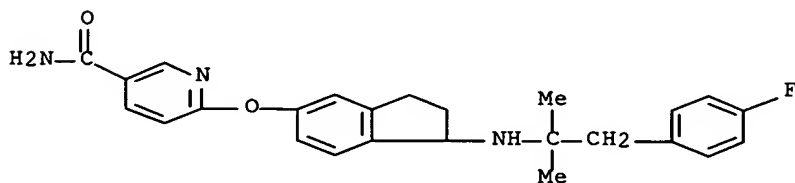
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CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-[3-(trifluoromethyl)phenyl]ethyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



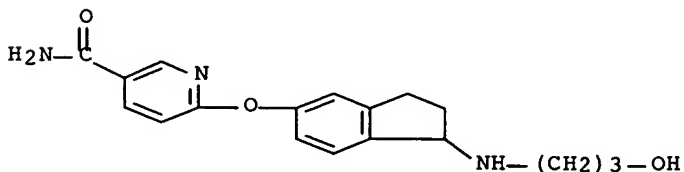
RN 762174-29-8 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[2-(4-fluorophenyl)-1,1-dimethylethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762174-31-2 HCAPLUS

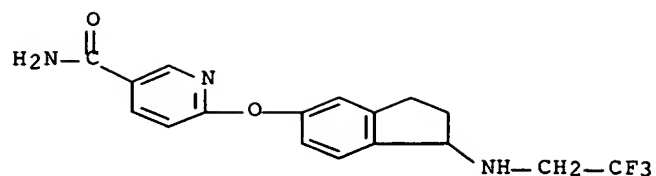
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(3-hydroxypropyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762174-33-4 HCAPLUS

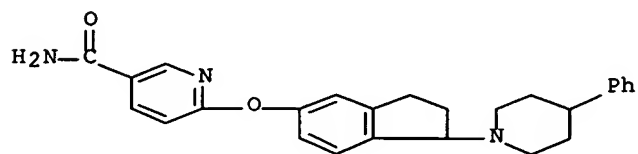
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(2,2,2-trifluoroethyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)





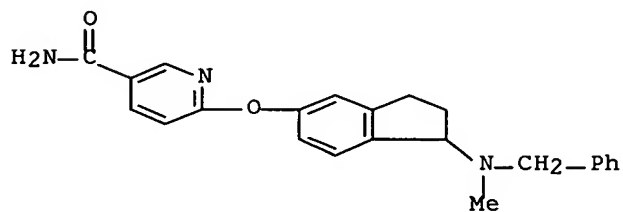
RN 762174-36-7 HCAPLUS

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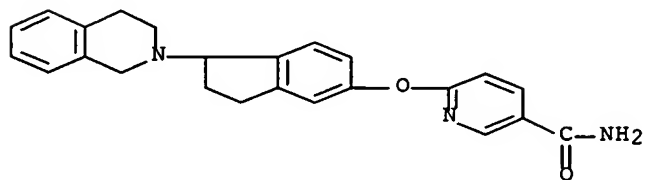
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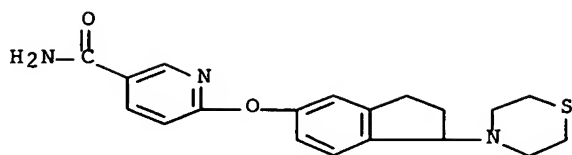
RN 762174-40-3 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-(3,4-dihydro-2(1H)-isoquinolinyl)-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



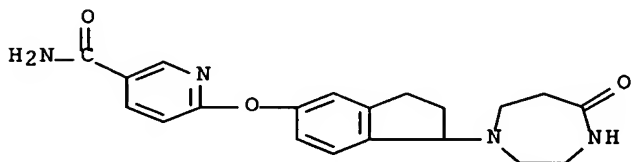
RN 762174-42-5 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-(4-thiomorpholinyl)-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



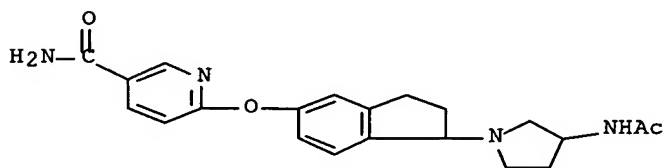
RN 762174-45-8 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-(hexahydro-5-oxo-1H-1,4-diazepin-1-yl)-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



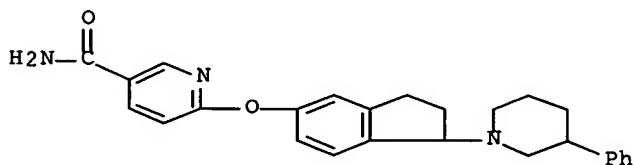
RN 762174-47-0 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[3-(acetylamino)-1-pyrrolidinyl]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



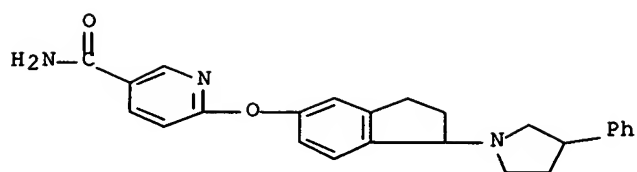
RN 762174-48-1 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-(3-phenyl-1-piperidinyl)-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



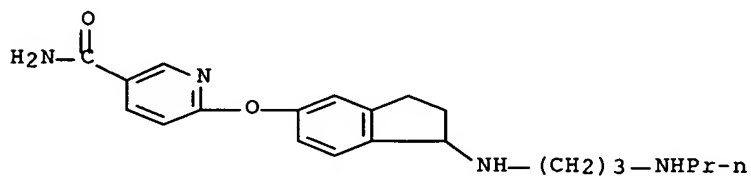
RN 762174-49-2 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-(3-phenyl-1-pyrrolidinyl)-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



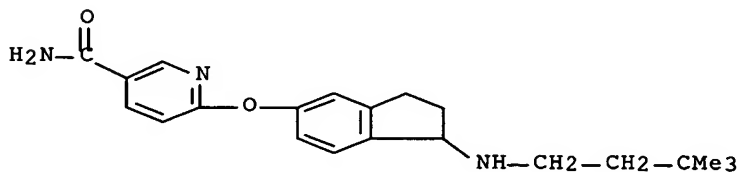
RN 762174-50-5 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[3-(propylamino)propyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



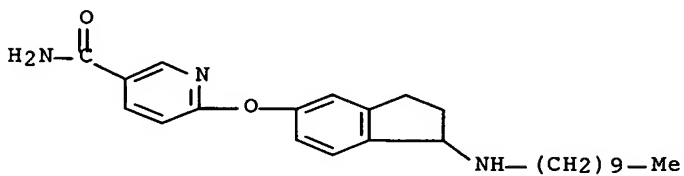
RN 762174-51-6 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[(3,3-dimethylbutyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



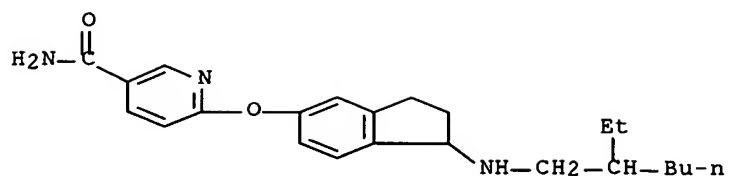
RN 762174-52-7 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-(decylamino)-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



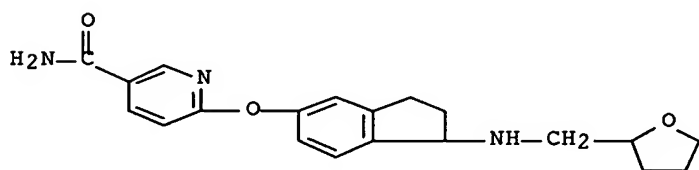
RN 762174-53-8 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[(2-ethylhexyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



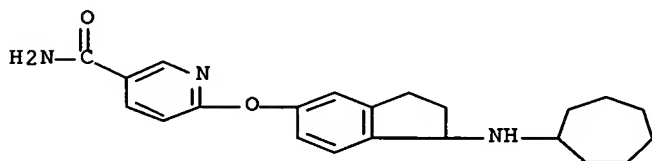
RN 762174-54-9 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[[(tetrahydro-2-furanyl)methyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



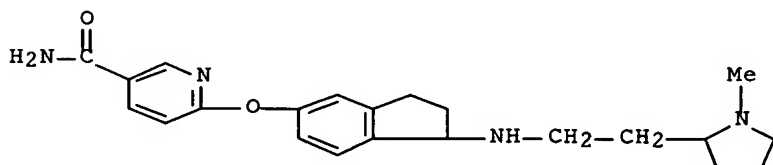
RN 762174-55-0 HCAPLUS

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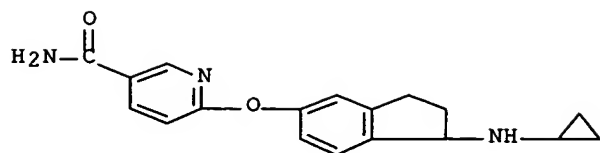
RN 762174-56-1 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-(1-methyl-2-pyrrolidinyl)ethyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



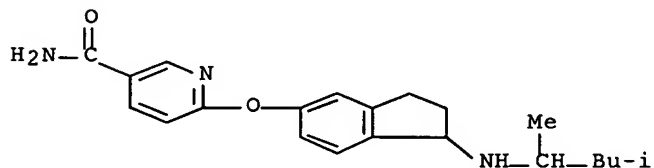
RN 762174-57-2 HCAPLUS

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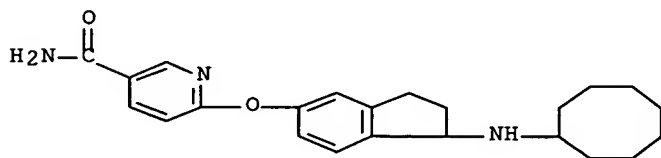
RN 762174-58-3 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[(1,3-dimethylbutyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



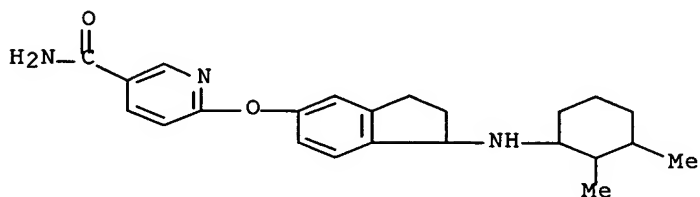
RN 762174-59-4 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-(cyclooctylamino)-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



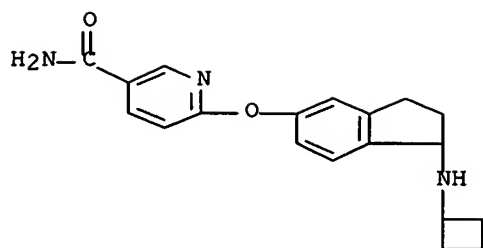
RN 762174-60-7 HCAPLUS

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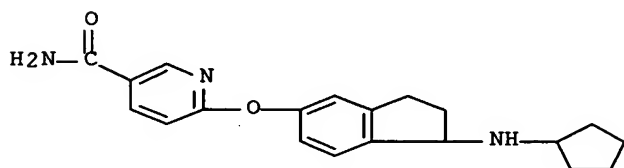
RN 762174-61-8 HCAPLUS

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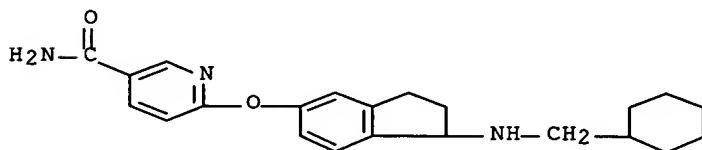
RN 762174-62-9 HCAPLUS

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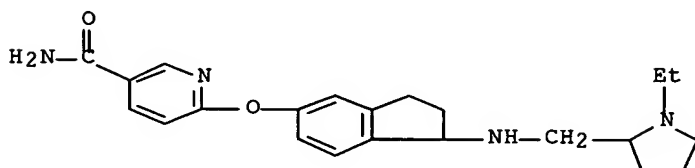
RN 762174-63-0 HCAPLUS

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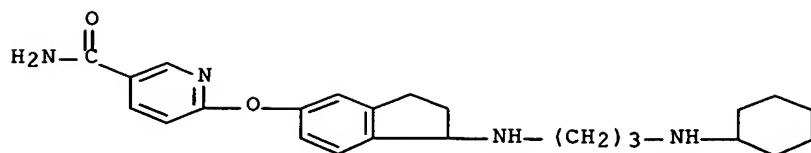
RN 762174-64-1 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[[1-ethyl-2-pyrrolidinyl)methyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



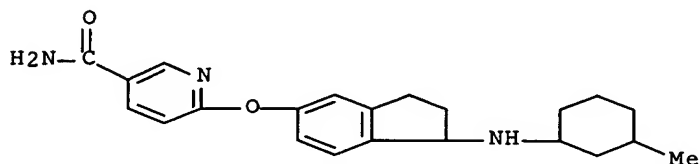
RN 762174-65-2 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[[3-(cyclohexylamino)propyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



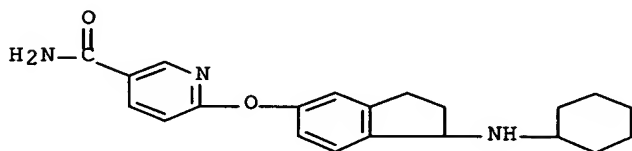
RN 762174-66-3 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(3-methylcyclohexyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



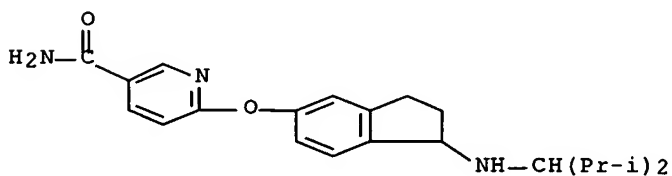
RN 762174-67-4 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-(cyclohexylamino)-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



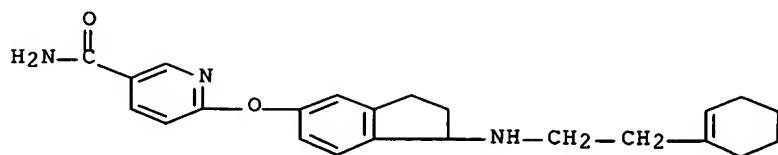
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CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[2-methyl-1-(1-methylethyl)propyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



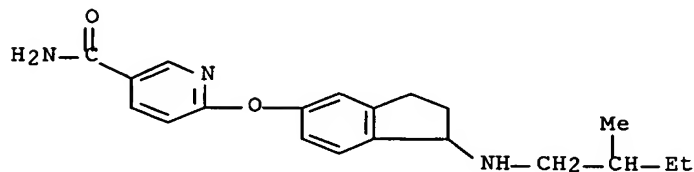
RN 762174-69-6 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[2-(1-cyclohexen-1-yl)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762174-70-9 HCAPLUS

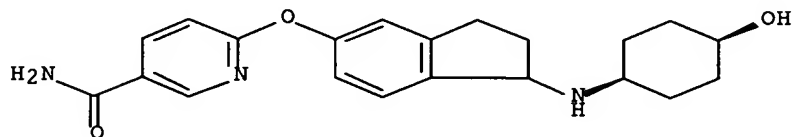
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(2-methylbutyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762174-71-0 HCAPLUS

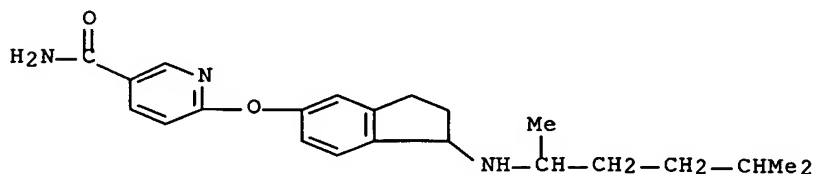
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(1S,2S)-2-methylbutyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 762174-72-1 HCAPLUS

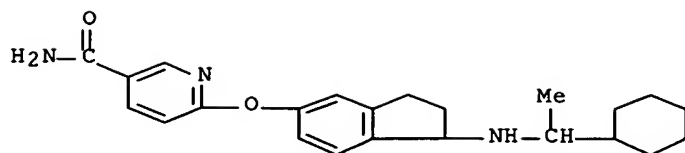
CN 3-Pyridinecarboxamide, 6-[[1-[(1,4-dimethylpentyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762174-73-2 HCAPLUS

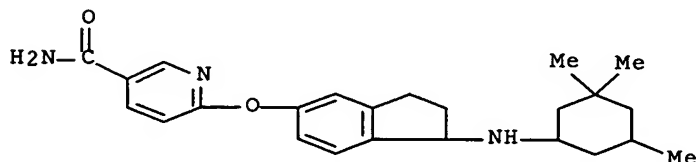
CN 3-Pyridinecarboxamide, 6-[[1-[(1-cyclohexylethyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)





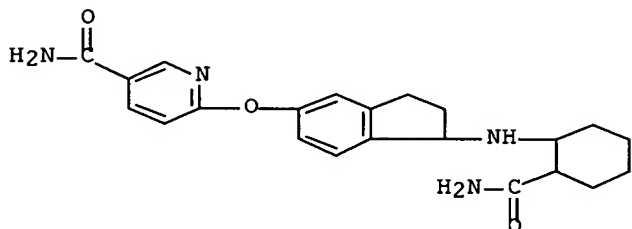
RN 762174-74-3 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(3,3,5-trimethylcyclohexyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



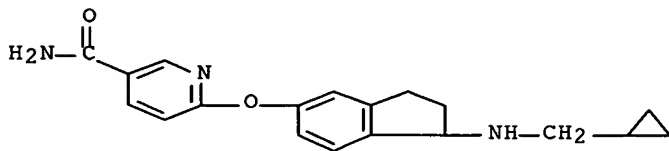
RN 762174-75-4 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[[2-(aminocarbonyl)cyclohexyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



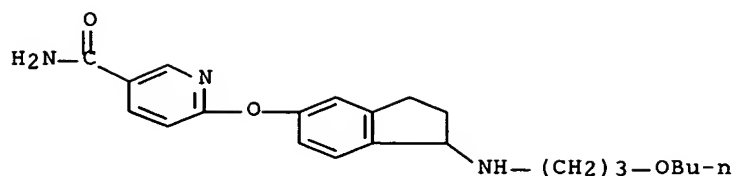
RN 762174-76-5 HCAPLUS

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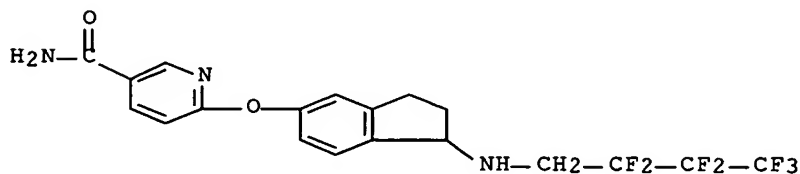
RN 762174-77-6 HCAPLUS

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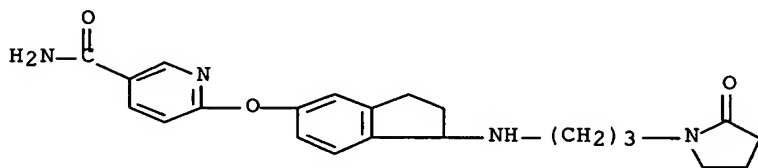
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CN 3-Pyridinecarboxamide, 6-[[1-[(2,2,3,3,4,4,4-heptafluorobutyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



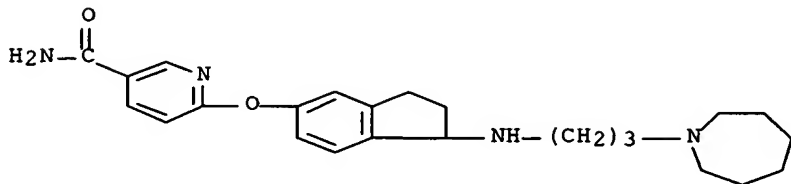
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CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



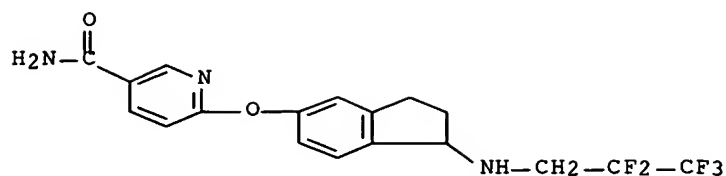
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RN 762174-81-2 HCAPLUS

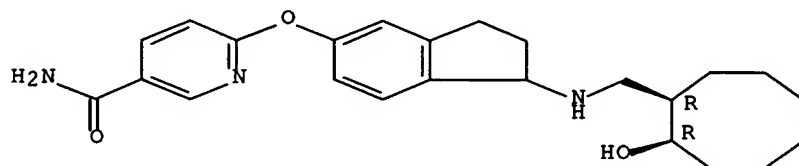
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[(2,2,3,3,3-pentafluoropropyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762174-82-3 HCAPLUS

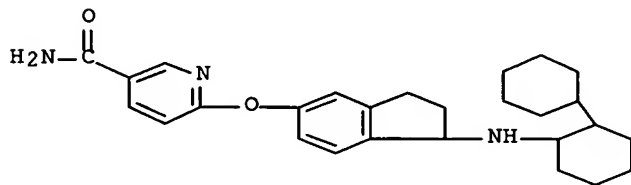
CN 3-Pyridinecarboxamide, 6-[[2,3-dihydro-1-[[[(1R,2R)-2-hydroxycyclooctyl]methyl]amino]-1H-inden-5-yl]oxy]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



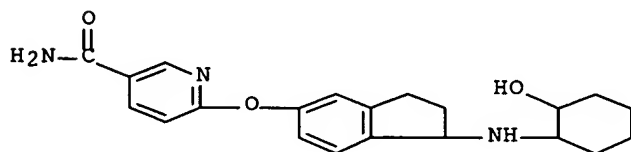
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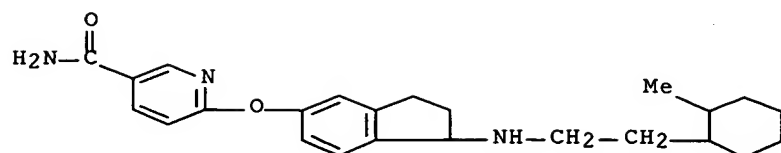
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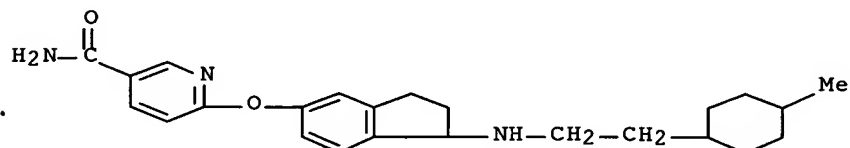
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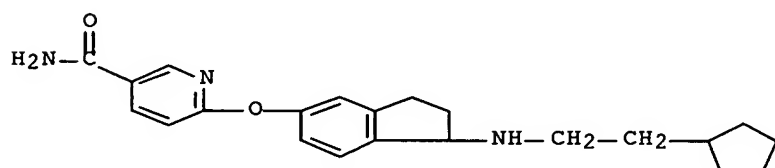
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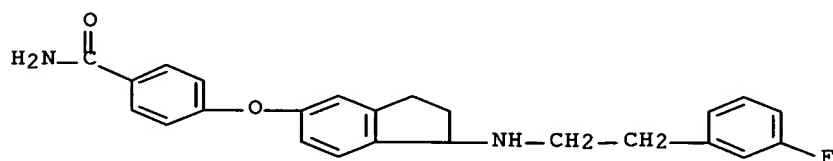
RN 762174-87-8 HCAPLUS

CN 3-Pyridinecarboxamide, 6-[[1-[(2-cyclopentylethyl)amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



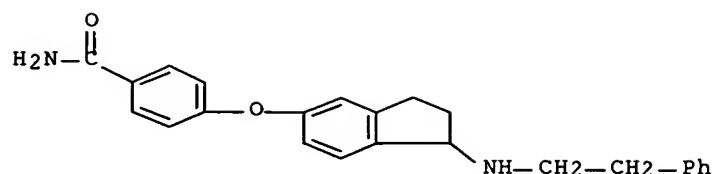
RN 762175-17-7 HCAPLUS

CN Benzamide, 4-[[1-[[2-(3-fluorophenyl)ethyl]amino]-2,3-dihydro-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 762175-18-8 HCAPLUS

CN Benzamide, 4-[[2,3-dihydro-1-[(2-phenylethyl)amino]-1H-inden-5-yl]oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:718521 HCAPLUS Full-text

DOCUMENT NUMBER: 141:225533

TITLE: Preparation of pyrimidines and triazines as human immunodeficiency virus replication inhibitors.

INVENTOR(S): Janssen, Paul Adriaan Jan; Guillemont, Jerome Emile Georges; Pasquier, Elisabeth Therese Jeanne; Heeres, Jan; Hertogs, Kurt; Bettens, Eva; Lewi, Paulus Joannes; De Jonge, Marc Rene; Koymans, Lucien Maria Henricus; Daeyaert, Frederik Frans Desire; Vinkers, Hendrik Maarten

PATENT ASSIGNEE(S): Tibotec Pharmaceuticals Ltd., Ire.; Arts, Frank Xavier Jozef Herwig; Arts, Theodora

SOURCE: PCT Int. Appl., 68 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

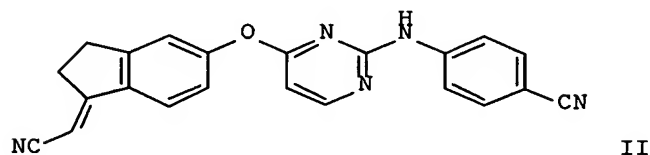
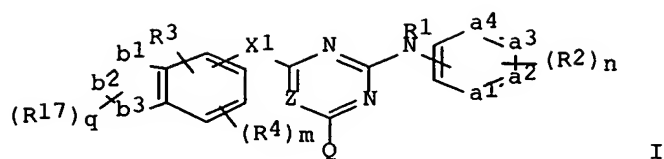
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004074261	A1	20040902	WO 2004-EP50175	20040220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2516699	AA	20040902	CA 2004-2516699	20040220
EP 1603887	A1	20051214	EP 2004-737251	20040220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			EP 2003-100411	A 20030220
			US 2003-475012P	P 20030602
			WO 2004-EP50175	W 20040220

OTHER SOURCE(S): MARPAT 141:225533

GI



AB Title compds. [I; ala2a3a4 = CH:CHCH:CH, N:CHCH:CH, N:CHN:CH, N:CHCH:N, N:NCH:CH; b1b2b3 = (CH2)3; n = 0-4; m = 0-3; q = 0-2; p = 1, 2; R1 = H, aryl, CHO, alkylcarbonyl, alkyl, alkoxy carbonyl, etc; R2 = OH, halo, alkyl, cyanoalkyl, cycloalkyl, alkenyl, haloalkenyl, cyanoalkenyl, alkynyl, haloalkynyl, cyanoalkynyl, etc.; X1 = NR5, NHNH, O, CO, alkylene, S, etc.; R3 = H, halo, alkyl, amino, aminocarbonyl, substituted alkyl, etc.; R4 = halo, OH, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, cyano, NO2, alkoxy carbonyl, etc.; R5 = H, aryl, CHO, alkylcarbonyl, alkyl, alkoxy carbonyl, etc; R17 = cyano, halo, OH, alkyl, cyanoalkyl, haloalkyl, alkenyl, cyanoalkenyl, haloalkenyl, alkynyl, cyanoalkynyl, haloalkynyl; :O, :S, :NH, etc.; Q = H, alkyl, polyhaloalkyl, amino, etc.; Z = CY; Y = H, OH, halo, alkyl, cycloalkyl, alkoxy, alkoxy carbonyl, aryl, alkenyl, haloalkenyl], were prepared. Thus, title compound (II) (preparation given) showed pEC50 = 8.7 against HIV-1 strain A.

IT **748150-47-2P 748150-52-9P**

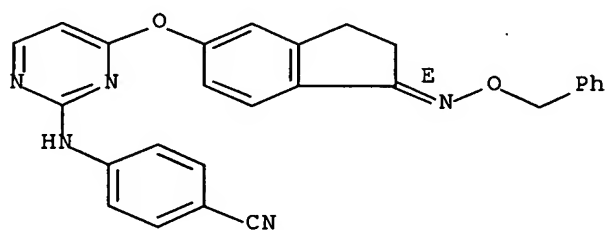
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidines and triazines as HIV replication inhibitors)

RN 748150-47-2 HCAPLUS

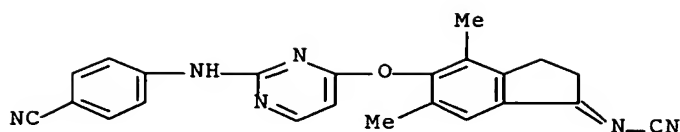
CN Benzonitrile, 4-[[4-[[[(1E)-2,3-dihydro-1-[(phenylmethoxy)imino]-1H-inden-5-yl]oxy]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 748150-52-9 HCAPLUS

CN Cyanamide, [5-[[2-[(4-cyanophenyl)amino]-4-pyrimidinyl]oxy]-2,3-dihydro-4,6-dimethyl-1H-inden-1-ylidene]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:453191 HCAPLUS Full-text

DOCUMENT NUMBER: 141:23546

TITLE: Preparation of 2,4-bis(phenylamino)pyrimidine derivatives for treating hyperproliferative disorders

INVENTOR(S): Wood, Jill E.; Bierer, Donald; Bear, Brian; Brennan, Catherine; Chandler, Brent; Chen, Gang; Chen, Yuanwei; Dixon, Julie; Fu, Wenlang; Guernon, Leatte; Liu, Donglei; McClure, Andrea; Miranda, Karl; Nagarathnam, Dhanapalan; Sibley, Robert; Turner, Michael; Verma, Sharad; Wang, Chunguang; Yi, Lin; Zhao, Jin; Zhu, Qingming

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046118	A2	20040603	WO 2003-US14294	20030506
WO 2004046118	A3	20040812		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-378329P P 20020506

OTHER SOURCE(S): MARPAT 141:23546

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [p = 0-2; X = alkyl, CF<sub>3</sub>, halo; R<sub>1</sub> = H, OH, halo, etc.; R<sub>2</sub> = H, S(O)<sub>2</sub>NH<sub>2</sub>, halo, etc.; R<sub>3</sub> = H, alkyl, halo, etc.; R<sub>4</sub> = H, halo, ethynyl, etc.; R<sub>5-6</sub> = H, halo, CF<sub>3</sub>; R<sub>7</sub> = H, halo, alkoxy; R<sub>8</sub> = H, alkyl, alkoxy, halo; R<sub>9</sub> = H, alkoxy] are prepared For instance, 4-fluoroaniline is alkylated with 5-bromo-2,4-dichloropyrimidine (THF, H<sub>2</sub>O, NaOAc); this intermediate is treated

10/721,015

with 3-(1-methyl-1H-pyrazol-3-yl)benzeneamine (t-BuOH, HCl) to give II.  
Compds. of the invention inhibit cell proliferation (no data).

IT 698996-27-9P 698996-29-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of 2,4-bis(phenylamino)pyrimidine derivs. for treating  
hyperproliferative disorders)

RN 698996-27-9 HCAPLUS

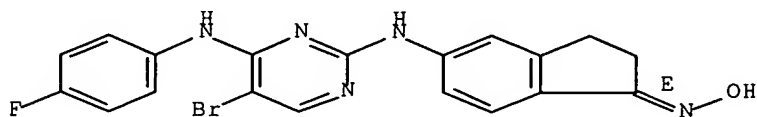
CN 1H-Inden-1-one, 5-[[5-bromo-4-[(4-fluorophenyl)amino]-2-pyrimidinyl]amino]-  
2,3-dihydro-, oxime, (1E)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 698996-26-8

CMF C19 H15 Br F N5 O

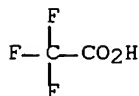
Double bond geometry as shown.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 698996-29-1 HCAPLUS

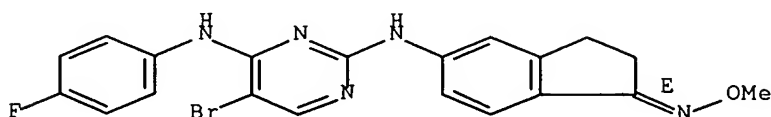
CN 1H-Inden-1-one, 5-[[5-bromo-4-[(4-fluorophenyl)amino]-2-pyrimidinyl]amino]-  
2,3-dihydro-, O-methyloxime, (1E)-, mono(trifluoroacetate) (9CI) (CA  
INDEX NAME)

CM 1

CRN 698996-28-0

CMF C20 H17 Br F N5 O

Double bond geometry as shown.

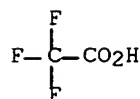




CM 2

CRN 76-05-1

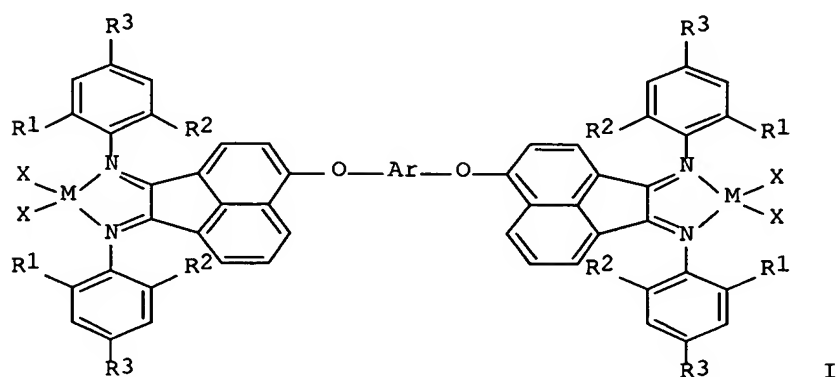
CMF C2 H F3 O2



L21 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:980376 HCAPLUS Full-text  
 DOCUMENT NUMBER: 140:28156  
 TITLE: Binuclear  $\alpha$ -diimine nickel olefin polymerization catalysts  
 INVENTOR(S): Li, Yuesheng; Liu, Jingyu; Zheng, Yi; Dai, Ke  
 PATENT ASSIGNEE(S): Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Peop. Rep. China  
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 27 pp.  
 CODEN: CNXXEV  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Chinese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1361184	A	20020731	CN 2000-136118	20001225
PRIORITY APPLN. INFO.:			CN 2000-136118	20001225
OTHER SOURCE(S):	MARPAT 140:28156			

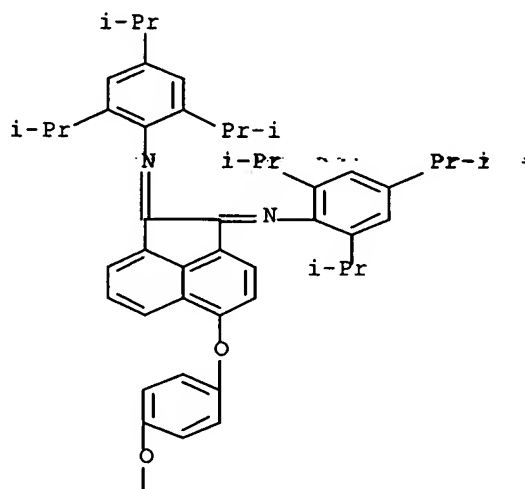
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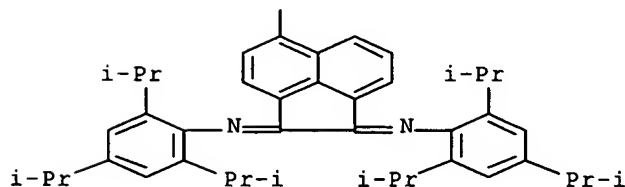
AB A binuclear  $\alpha$ -diimine nickel complex having the formula I was prepared and used for producing branched and high mol. weight polyethylene, where M = Ni, X = Br or Cl, R1 and R2 = H, Cl, Me, Et, CHMe2, CMe3 or CF3, R3 = H, Cl, Me or CHMe2, Ar = phenylene, substituted phenylene, biphenylene, naphthylene or diphenylmethylenes.

IT 634205-72-4P 634205-73-5P 634205-75-7P  
 634205-76-8P 634205-77-9P 634205-78-0P  
 634205-79-1P 634205-80-4P 634205-81-5P  
 634205-82-6P 634205-83-7P 634205-84-8P  
 634205-85-9P 634205-86-0P 634205-87-1P  
 634205-88-2P 634205-89-3P 634205-90-6P  
 634205-91-7P 634205-92-8P 634205-93-9P  
 634205-94-0P 634205-95-1P 634205-96-2P  
 634205-97-3P 634205-98-4P 634205-99-5P  
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (ligands for the synthesis of binuclear  $\alpha$ -diimine nickel olefin  
 polymerization catalysts)  
 RN 634205-72-4 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[1,4-phenylenebis(oxy-5-acenaphthylenyl-1,2-  
 diylidene)]tetrakis[2,4,6-tris(1-methylethyl)- (9CI) (CA INDEX NAME)

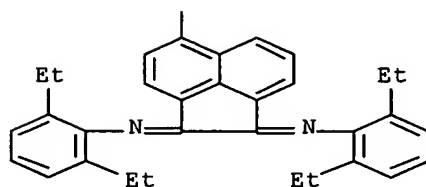
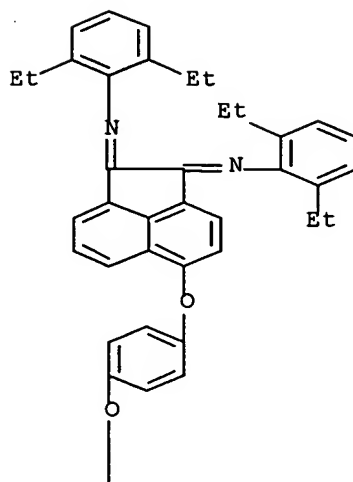
PAGE 1-A



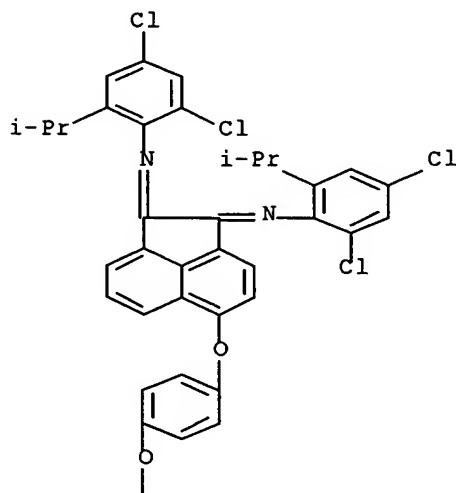
PAGE 2-A



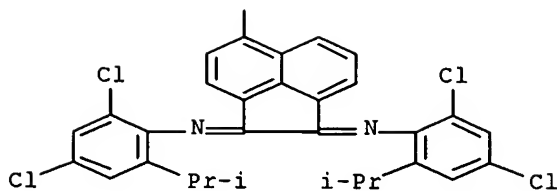
RN 634205-73-5 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[1,4-phenylenebis(oxy-5-acenaphthylenyl-1,2-  
 diylidene)]tetrakis[2,6-diethyl- (9CI) (CA INDEX NAME)



RN 634205-75-7 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[1,4-phenylenebis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,4-dichloro-6-(1-methylethyl)- (9CI) (CA INDEX NAME)



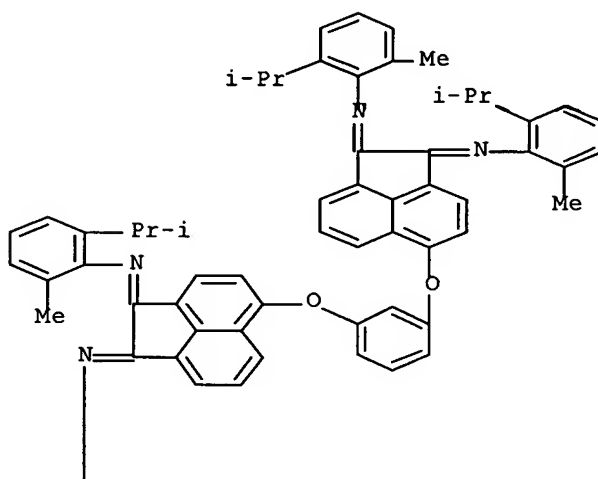
PAGE 2-A



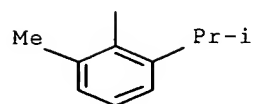
RN 634205-76-8 HCAPLUS

CN Benzenamine, N,N',N'',N'''-[1,3-phenylenebis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2-methyl-6-(1-methylethyl)- (9CI) (CA INDEX NAME)

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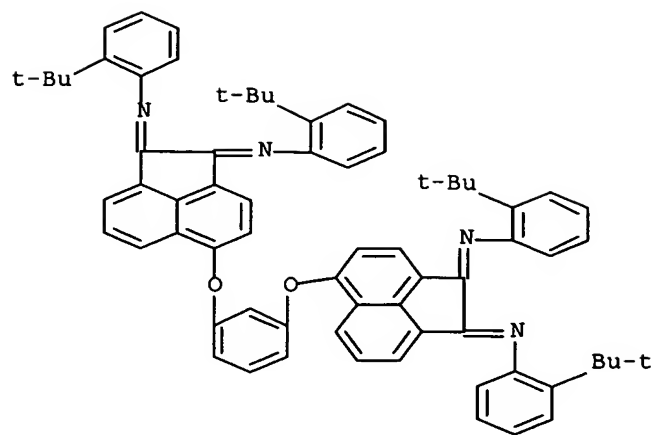


PAGE 2-A



RN 634205-77-9 HCAPLUS

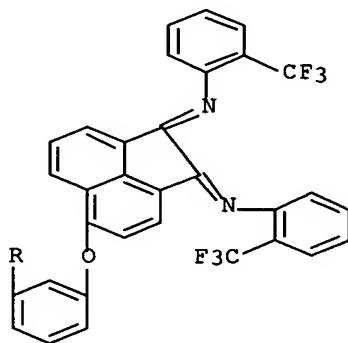
CN Benzenamine, N,N',N'',N'''-[1,3-phenylenebis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



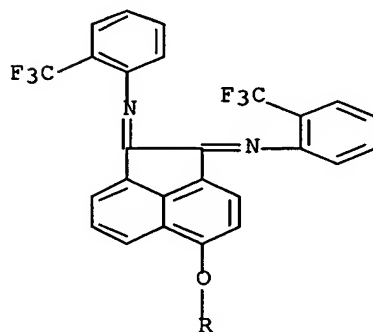
RN 634205-78-0 HCAPLUS

CN Benzenamine, N,N',N'',N'''-[1,3-phenylenebis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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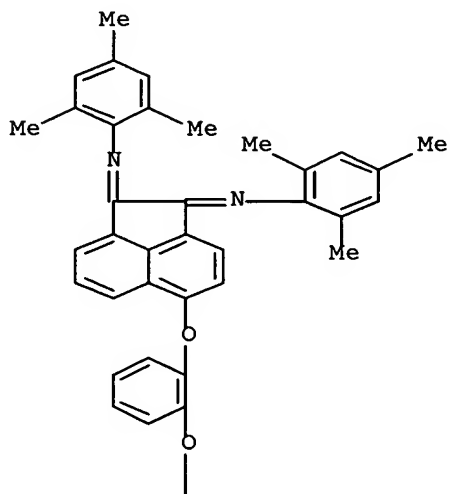


RN 634205-79-1 HCAPLUS

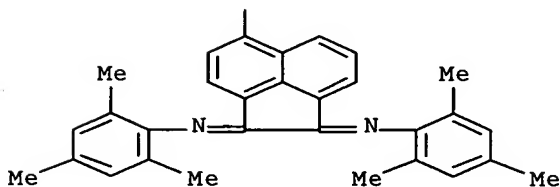
10/721,015

CN Benzenamine, N,N',N'',N'''-[1,2-phenylenebis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,4,6-trimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A

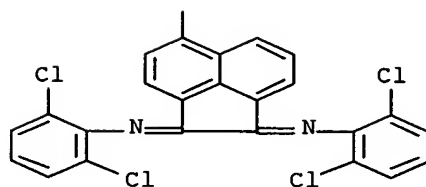
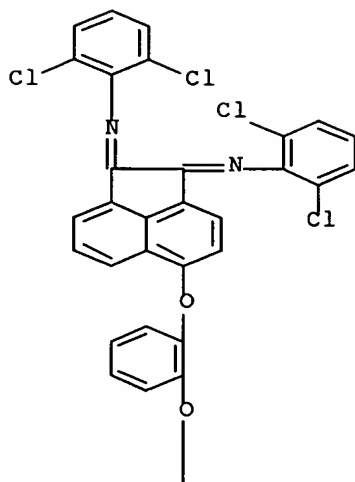


PAGE 2-A

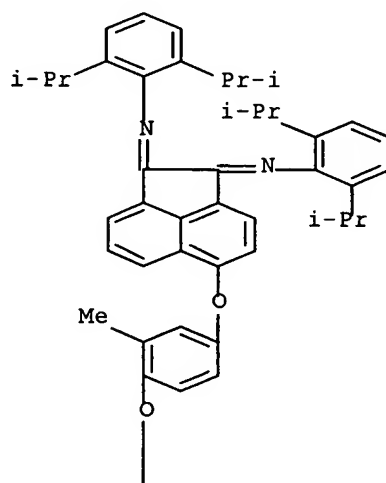


RN 634205-80-4 HCAPLUS

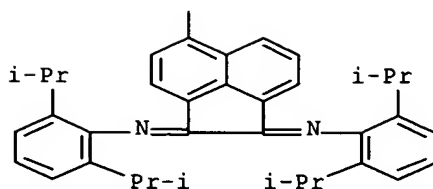
CN Benzenamine, N,N',N'',N'''-[1,2-phenylenebis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-dichloro- (9CI) (CA INDEX NAME)



RN 634205-81-5 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[ (2-methyl-1,4-phenylene)bis(oxy-5-acenaphthylene-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

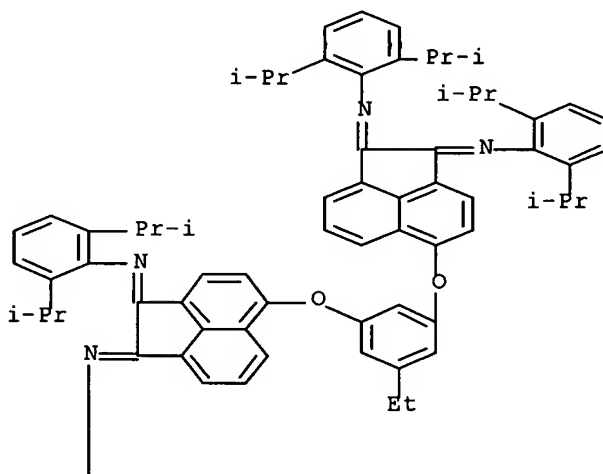


PAGE 2-A

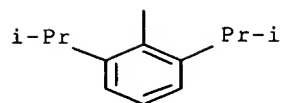


RN 634205-82-6 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[(5-ethyl-1,3-phenylene)bis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

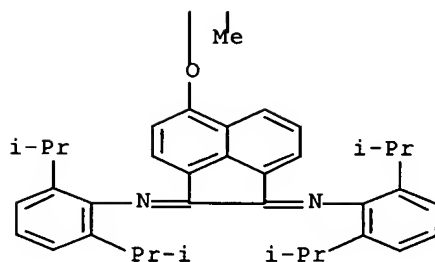
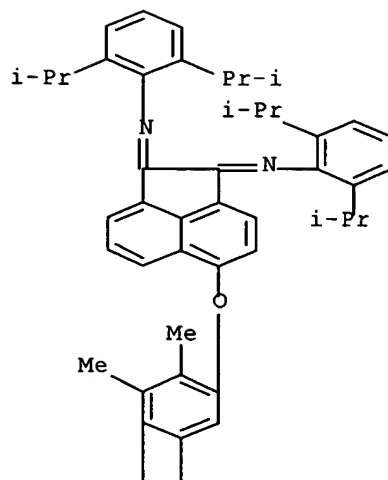


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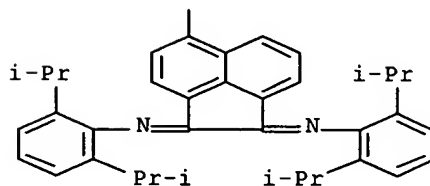
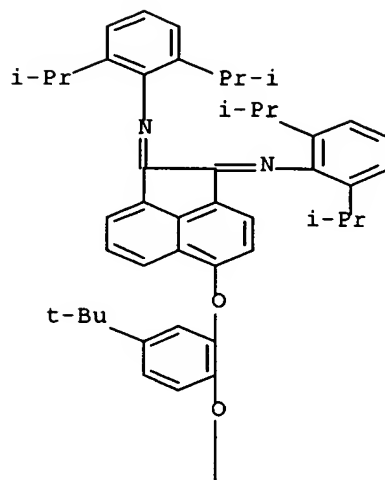


RN 634205-83-7 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[(2,3,5-trimethyl-1,4-phenylene)bis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

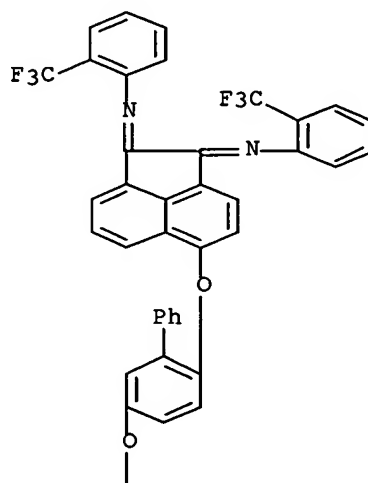




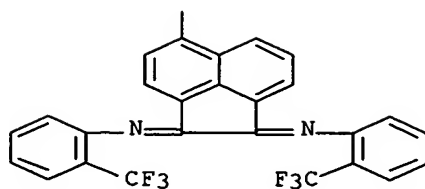
RN 634205-84-8 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[[4-(1,1-dimethylethyl)-1,2-phenylene]bis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 634205-85-9 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[1,1'-biphenyl]-2,5-diylbis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



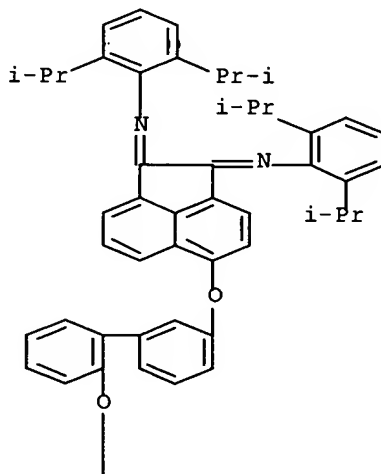
PAGE 2-A



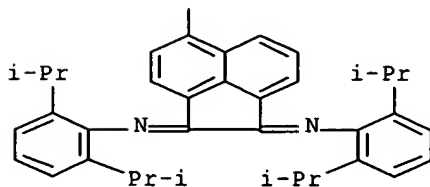
RN 634205-86-0 HCAPLUS

CN Benzenamine, N,N',N'',N'''-[1,1'-biphenyl]-2,3'-diylbis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

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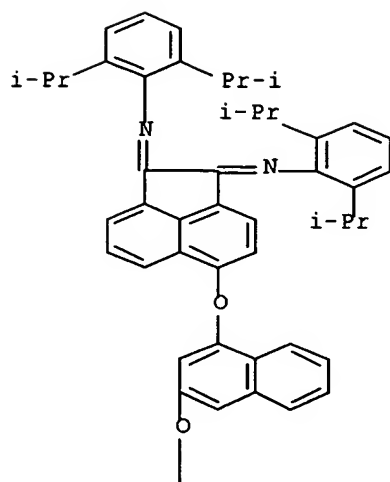
PAGE 2-A



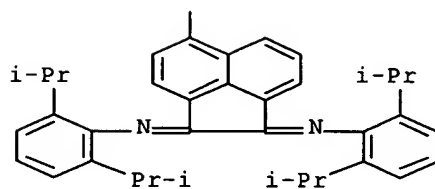
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CN Benzenamine, N,N',N'',N'''-[1,3-naphthalenediylbis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

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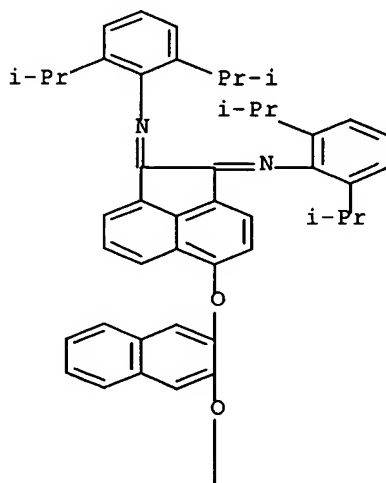


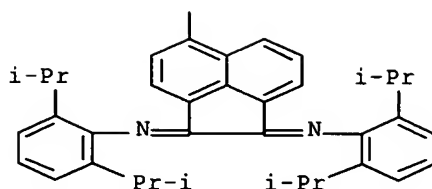
PAGE 2-A



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 CN Benzenamine, N,N',N'',N'''-[2,3-naphthalenediylbis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

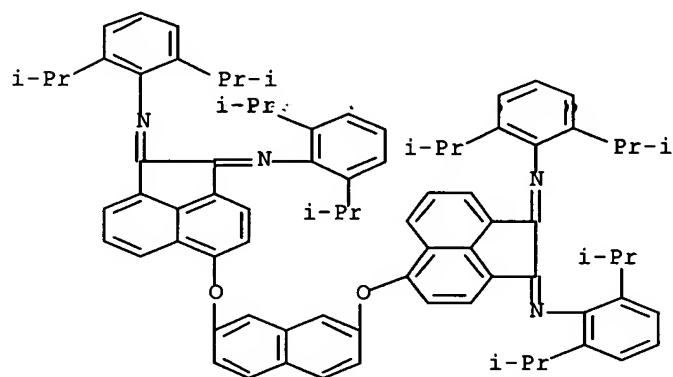
PAGE 1-A





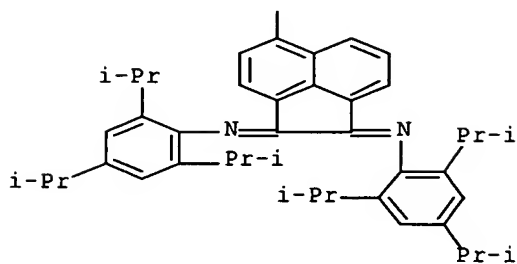
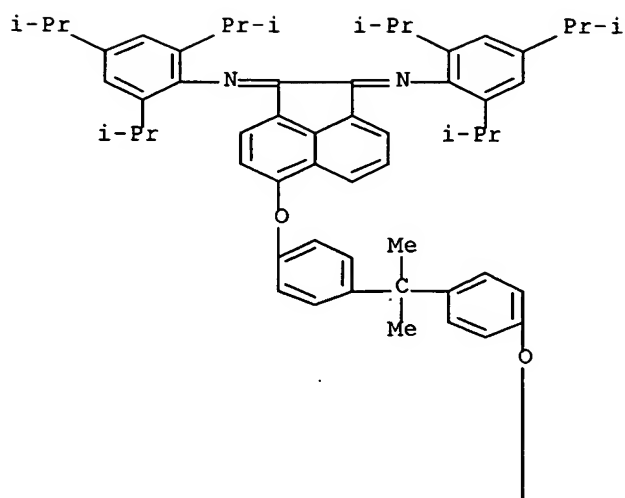
RN 634205-89-3 HCAPLUS

CN Benzenamine, N,N',N'',N'''-[2,7-naphthalenediylbis(oxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

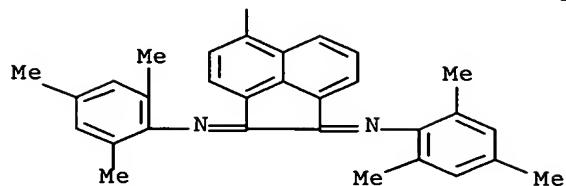
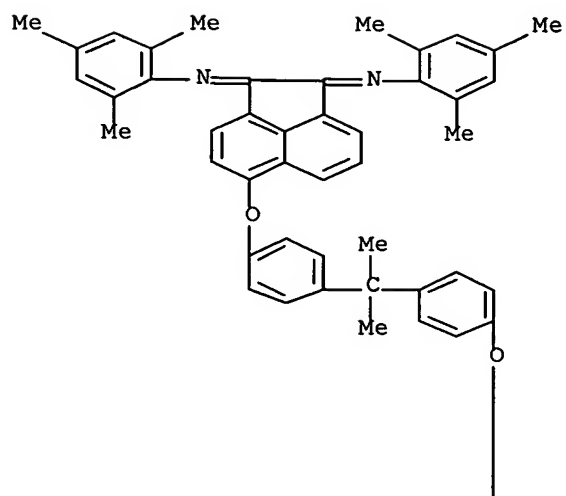


RN 634205-90-6 HCAPLUS

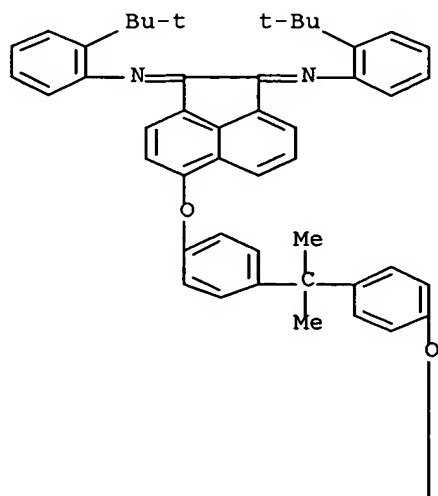
CN Benzenamine, N,N',N'',N'''-[(1-methylethylidene)bis(4,1-phenyleneoxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,4,6-tris(1-methylethyl)- (9CI) (CA INDEX NAME)



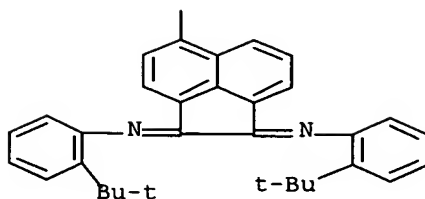
RN 634205-91-7 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[(1-methylethylidene)bis(4,1-phenyleneoxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,4,6-trimethyl- (9CI) (CA INDEX NAME)



RN 634205-92-8 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[(1-methylethylidene)bis(4,1-phenyleneoxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



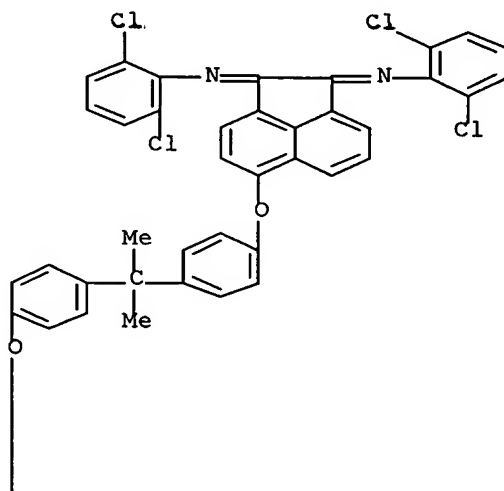
PAGE 2-A



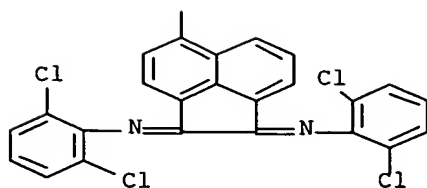
RN 634205-93-9 HCAPLUS

CN Benzenamine, N,N',N'',N'''-[(1-methylethylidene)bis(4,1-phenyleneoxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-dichloro- (9CI) (CA INDEX NAME)]

PAGE 1-A



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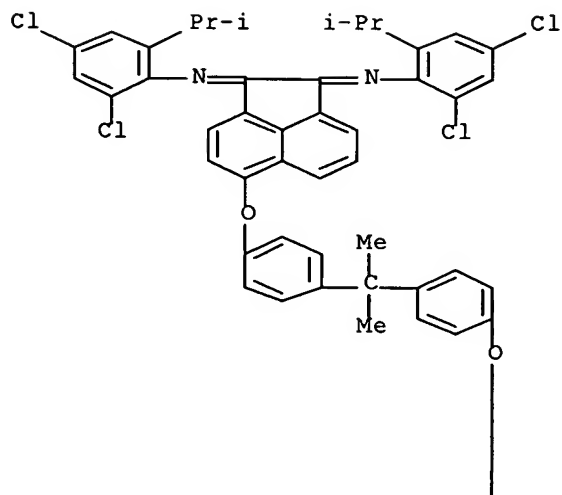
RN 634205-94-0 HCAPLUS

CN Benzenamine, N,N',N'',N'''-[(1-methylethylidene)bis(4,1-phenyleneoxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,4-dichloro-6-(1-methylethyl)-

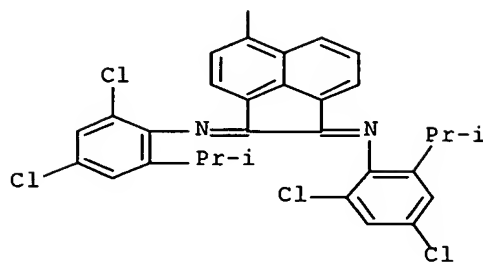


(9CI) (CA INDEX NAME)

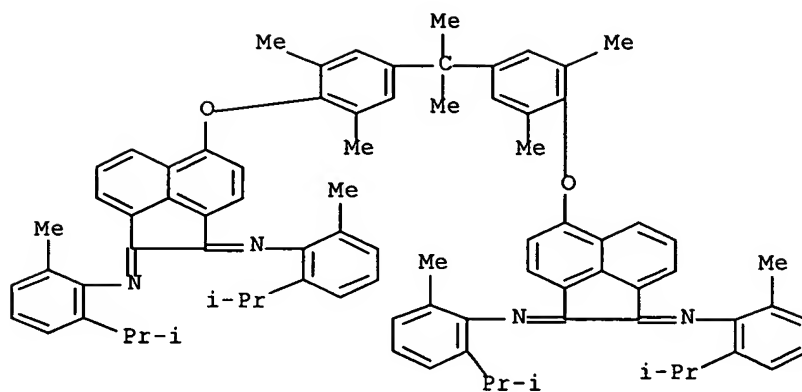
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PAGE 2-A

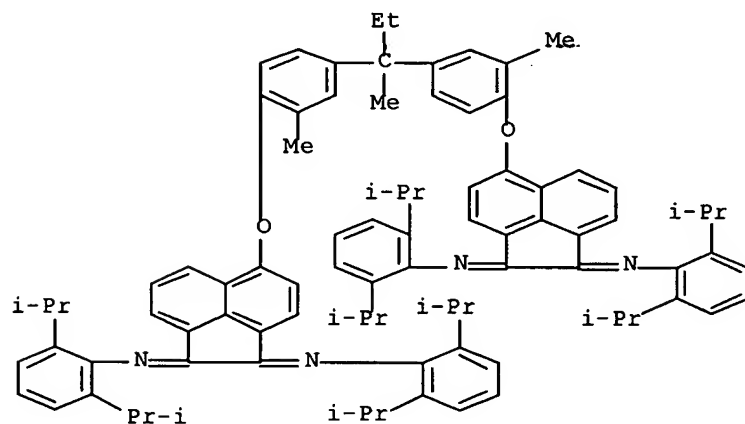


RN 634205-95-1 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[(1-methylethylidene)bis[(2,6-dimethyl-4,1-phenylene)oxy-5-acenaphthylenyl-1,2-diylidene]]tetrakis[2-methyl-6-(1-methylethyl)- (9CI) (CA INDEX NAME)



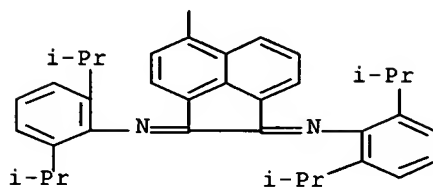
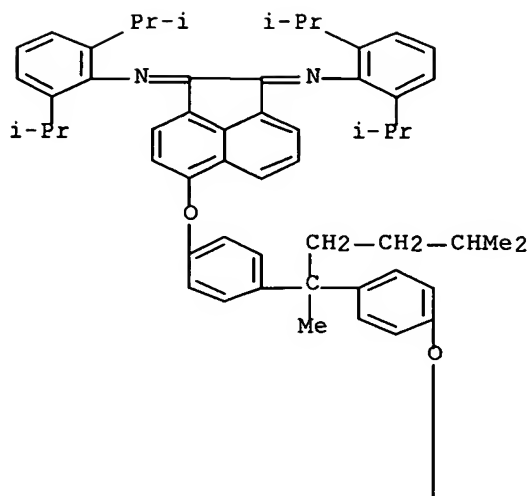
RN 634205-96-2 HCAPLUS

CN Benzenamine, N,N',N'',N'''-[(1-methylpropylidene)bis[(2-methyl-4,1-phenylene)oxy-5-acenaphthylenyl-1,2-diylidene]]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

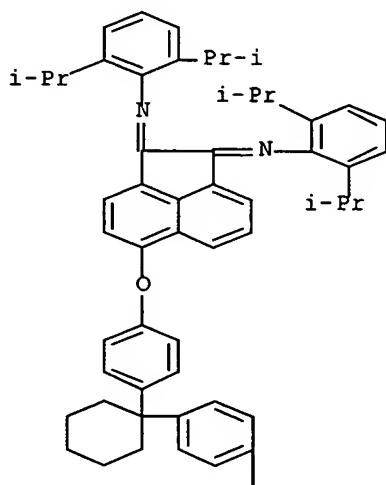


RN 634205-97-3 HCAPLUS

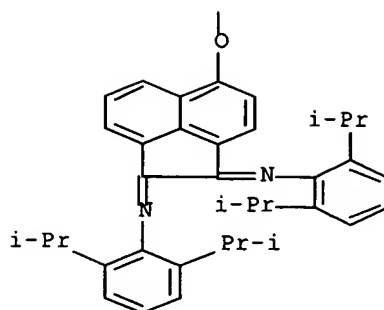
CN Benzenamine, N,N',N'',N'''-[(1,4-dimethylpentylidene)bis(4,1-phenyleneoxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 634205-98-4 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[cyclohexylidenebis(4,1-phenyleneoxy-5-acenaphthylenyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)-(9CI) (CA INDEX NAME)

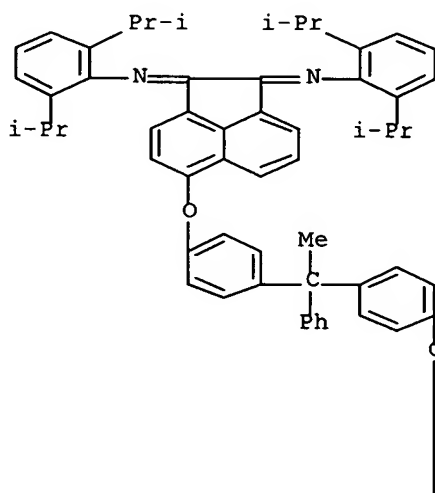


PAGE 2-A

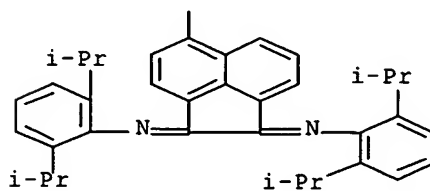


RN 634205-99-5 HCAPLUS  
 CN Benzenamine, N,N',N'',N'''-[(1-phenylethylidene)bis(4,1-phenyleneoxy-5-acenaphthyl-1,2-diylidene)]tetrakis[2,6-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L21 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:319711 HCAPLUS Full-text  
 DOCUMENT NUMBER: 138:338153  
 TITLE: Preparation of 2'-methyl-5'-(1,3,4-oxadiazol-2-yl)-  
 1,1'-biphenyl-4-carboxamides as p38 kinase inhibitors  
 INVENTOR(S): Angell, Richard Martyn; Bamborough, Paul; Cockerill,  
 George Stuart; Walker, Ann Louise  
 PATENT ASSIGNEE(S): Glaxo Group Limited, UK  
 SOURCE: PCT Int. Appl., 61 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032986	A1	20030424	WO 2002-EP11569	20021016
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1435949	A1	20040714	EP 2002-777313	20021016
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
JP 2005507910	T2	20050324	JP 2003-535789	20021016
US 2004266839	A1	20041230	US 2004-492713	20040415
PRIORITY APPLN. INFO.:			GB 2001-24936	A 20011017
			WO 2002-EP11569	W 20021016
OTHER SOURCE(S):	MARPAT 138:338153			
GI				

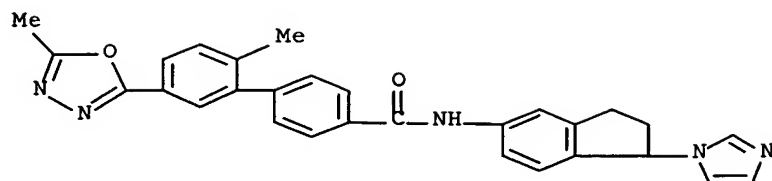
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I; R1 = (un)substituted Ph; R2 = H, alkyl, (CH2)pcycloalkyl; R3 = II (wherein R4 = H, alkyl); U = Me, halo; X, Y = H, Me, halo; m = 0-4; n = 0-2; p = 0-2], useful as pharmaceuticals, particularly as p38 kinase inhibitors, were prepared E.g., 6-step synthesis of the carboxamide III, starting from 3-bromo-4-methylbenzoic acid, was given.

IT **515153-39-6P**  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 2'-methyl-5'-(1,3,4-oxadiazol-2-yl)-1,1'-biphenyl-4-carboxamides as p38 kinase inhibitors)

RN 515153-39-6 HCAPLUS

CN [1,1'-Biphenyl]-4-carboxamide, N-[2,3-dihydro-1-(1H-imidazol-1-yl)-1H-inden-5-yl]-2'-methyl-5'-(5-methyl-1,3,4-oxadiazol-2-yl)- (9CI) (CA INDEX NAME)

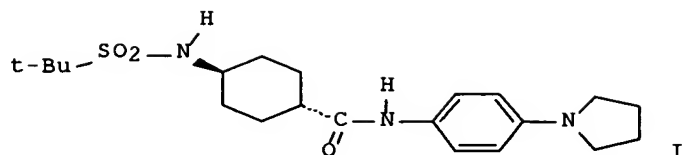


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2001:396661 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:19547  
 TITLE: Preparation of sulfonamides and sulfinamides as NPY Y5 antagonists  
 INVENTOR(S): Kawanishi, Yasuyuki; Takenaka, Hideyuki; Hanasaki, Kohji; Okada, Tetsuo  
 PATENT ASSIGNEE(S): Shionogi & Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 273 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001037826	A1	20010531	WO 2000-JP8197	20001121
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2389681	AA	20010531	CA 2000-2389681	20001121
AU 2001014186	A5	20010604	AU 2001-14186	20001121
AU 780790	B2	20050414		
BR 2000015843	A	20020827	BR 2000-15843	20001121
EP 1249233	A1	20021016	EP 2000-976387	20001121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NZ 519070	A	20050826	NZ 2000-519070	20001121
RU 2264810	C2	20051127	RU 2002-117021	20001121
ZA 2002003306	A	20030425	ZA 2002-3306	20020425
US 6699891	B1	20040302	US 2002-111981	20020501
NO 2002002481	A	20020726	NO 2002-2481	20020524
US 2004176462	A1	20040909	US 2003-747034	20031230
US 2004180964	A1	20040916	US 2003-747359	20031230
PRIORITY APPLN. INFO.:			JP 1999-336469	A 19991126
			JP 1999-353786	A 19991214
			WO 2000-JP8197	W 20001121
			US 2002-111981	A3 20020501
OTHER SOURCE(S):			MARPAT 135:19547	

GI



AB The title compds. R1S(O)nN(R2)XYZ [R1 represents lower alkyl, cycloalkyl, etc.; R2 represents hydrogen, lower alkyl, etc.; n is 1 or 2; X represents lower alkylene, lower alkenylene, arylene, cycloalkylene, etc.; Y represents CONR7, CSNR7, NR7CO, NR7CS, etc. (wherein R7 represents hydrogen or lower alkyl); and Z represents lower alkyl, an optionally substituted hydrocarbon ring, an optionally substituted heterocycle, etc.] are prepared. In an in vitro test for affinity for the neuropeptide Y5 receptors, the title compound I showed the IC50 value of 0.4 nM. Formulations are given.

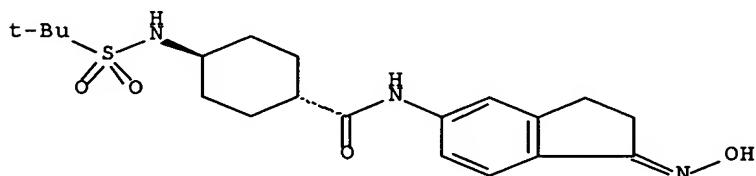
IT 342575-75-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of sulfonamides and sulfinamides as NPY Y5 antagonists).

RN 342575-75-1 HCAPLUS

CN Cyclohexanecarboxamide, N-[2,3-dihydro-1-(hydroxyimino)-1H-inden-5-yl]-4-[[ (1,1-dimethylethyl)sulfonyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry unknown.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:505662 HCAPLUS Full-text

DOCUMENT NUMBER: 131:144612

TITLE: Preparation of N-cycloalkylpiperazines as M2 muscarinic receptor antagonists

INVENTOR(S): Kozlowski, Joseph A.; Lowe, Derek B.; Chang, Wei K.; Dugar, Sundee

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: U.S., 20 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

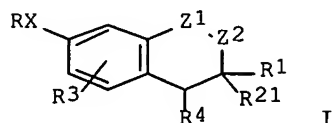
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5935958	A	19990810	US 1997-883183	19970626
PRIORITY APPLN. INFO.:			US 1996-21171P	P 19960701
OTHER SOURCE(S):	MARPAT	131:144612		

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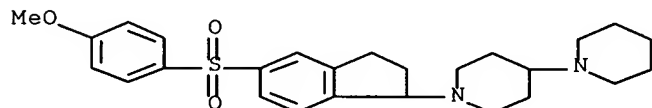
AB Title compds. [I; R = 2-pyrimidinyl, (un)substituted Ph, etc.; R1, R21 = H, (cyclo)alk(en)yl, phenylalkyl, etc.; R3 = H or 1 or 2 of halo, alkyl, alkoxy, etc.; R4 = ZR2; R2 = cycloalk(en)yl, (un)substituted piperidino, etc.; X = O, SOO-2, CO, CH2, NH, etc.; Z = (un)substituted piperazine-1,4-diyl, (un)substituted (4-alkyl)piperidine-1,4-diyl; Z1 = O, SOO-2, CH2; Z2 = bond or (CH2)1-3] were prepared. Thus, 2-(HO)C6H4OH was cyclocondensed with ClCH2CH2COCl and the product etherified by 4-FC6H4NO2 to give, in 3 addnl. steps, I [R = C6H4(NO2)-4, R1, R21, R3 = H, R4 = 4-cyclohexyl-1-piperazinyl, X, Z1 = O, Z2 = CH2]. Data for biol. activity of I were given.

IT 201745-57-5P 201745-59-7P 201745-61-1P  
201745-64-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of N-cycloalkylpiperazines as M2 muscarinic receptor antagonists)

RN 201745-57-5 HCAPLUS

CN 1,4'-Bipiperidine, 1'-[2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]- (9CI) (CA INDEX NAME)

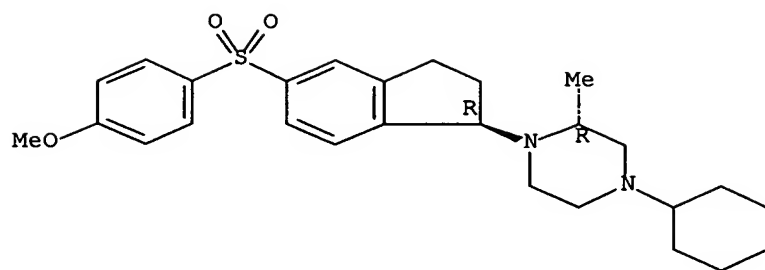


RN 201745-59-7 HCAPLUS

CN Piperazine, 4-cyclohexyl-1-[(1R)-2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]-2-methyl-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



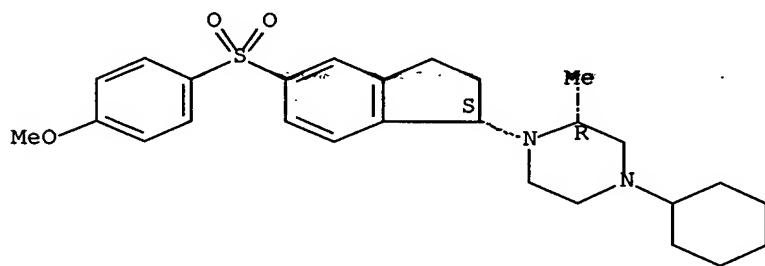


● HCl

RN 201745-61-1 HCAPLUS

CN Piperazine, 4-cyclohexyl-1-[(1S)-2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]-2-methyl-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

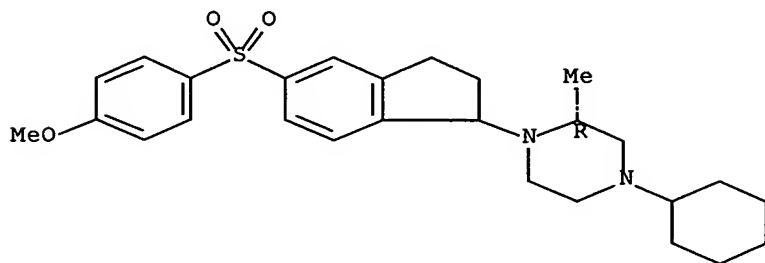


● HCl

RN 201745-64-4 HCAPLUS

CN Piperazine, 4-cyclohexyl-1-[2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

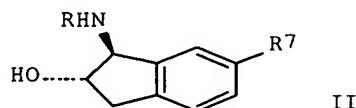
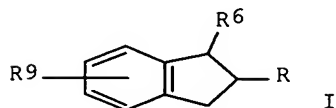
21

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:105937 HCAPLUS Full-text  
 DOCUMENT NUMBER: 128:153932  
 TITLE: Preparation of N-indanylbenzenesulfonamides and analogs as potassium channel blockers  
 INVENTOR(S): Castle, Neil Alexander; Hollinshead, Sean Patrick; Hughes, Philip Floyd; Mendoza, Jose Serafin; Wilson, Joseph Wendell; Amato, George; Beaudoin, Serge; et al.  
 PATENT ASSIGNEE(S): Icagen, Inc., USA; Eli Lilly and Company  
 SOURCE: PCT Int. Appl., 85 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9804521	A1	19980205	WO 1997-US12559	19970723
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6083986	A	20000704	US 1997-893160	19970715
CA 2261814	AA	19980205	CA 1997-2261814	19970723
AU 9738035	A1	19980220	AU 1997-38035	19970723
AU 734711	B2	20010621		
EP 923543	A1	19990623	EP 1997-934996	19970723
EP 923543	B1	20030924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9710587	A	20001031	BR 1997-10587	19970723
JP 2002513385	T2	20020508	JP 1998-508884	19970723
IL 128205	A1	20030917	IL 1997-128205	19970723
AT 250571	E	20031015	AT 1997-934996	19970723
ZA 9706640	A	19980302	ZA 1997-6640	19970725
KR 2000029605	A	20000525	KR 1999-700669	19990126
HK 1020334	A1	20040528	HK 1999-105493	19991126
PRIORITY APPLN. INFO.:			US 1996-22547P	P 19960726
			US 1997-893160	A 19970715
			WO 1997-US12559	W 19970723
OTHER SOURCE(S):			MARPAT 128:153932	
GI				



AB Title compds. [I; R = H, OR5, (di)(alkyl)amino, alkoxycarbonylamino, etc.; R5 = H, (CH2)mR8, CO(CH2)mR8; R6 = NR3Z2Z1R1; R1 = H, alkyl, (hetero)aryl, etc.; R3 = H or Me; R8 = (di)(alkyl)amino, CO2H, alkoxycarbonyl, etc.; R9 = R2Z3Z4NR4; R2 = alkyl, heterocyclyl, (hetero)aryl, etc.; R4 = H or Me; Z1 = CO

or SO<sub>2</sub>; Z<sub>2</sub> = bond, O, CH<sub>2</sub>, NH, CH:CH; Z<sub>3</sub> = bond, O, CH<sub>2</sub>, NH, CH:CH, etc.; Z<sub>4</sub> = CO, CS, SO<sub>2</sub>; m = 1-5] were prepared. Thus, indanamine II (R = H, R<sub>7</sub> = NO<sub>2</sub>) (preparation given) was amidated by 4-EtC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>Cl and the reduced product amidated by 3-(MeO)C<sub>6</sub>H<sub>4</sub>COCl to give II [R = 4-EtC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>, R<sub>7</sub> = 3-(MeO)C<sub>6</sub>H<sub>4</sub>CONH]. Data for biol. activity of I were given.

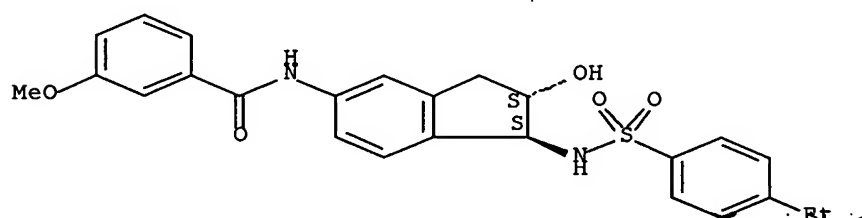
IT 202749-03-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of N-indanylbzenesulfonamides and analogs as potassium channel blockers)

RN 202749-03-9 HCAPLUS

CN Benzamide, N-[1-[[[(4-ethylphenyl)sulfonyl]amino]-2,3-dihydro-2-hydroxy-1H-inden-5-yl]-3-methoxy-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:55628 HCAPLUS Full-text

DOCUMENT NUMBER: 128:114963

TITLE: Preparation of piperazine and piperidine derivatives as muscarinic antagonists

INVENTOR(S): Kozlowski, Joseph A.; Lowe, Derek B.; Chang, Wei K.; Dugar, Sundeeep

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

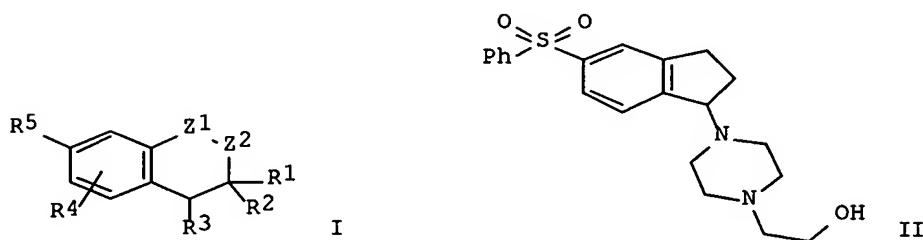
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9800412	A1	19980108	WO 1997-US10696	19970626
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2258044	AA	19980108	CA 1997-2258044	19970626
AU 9734953	A1	19980121	AU 1997-34953	19970626
AU 717431	B2	20000323		

EP 912534 A1 19990506 EP 1997-931281 19970626  
 EP 912534 B1 20020925  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,  
 LT, LV, FI, RO  
 NZ 333322 A 20000623 NZ 1997-333322 19970626  
 JP 2000514060 T2 20001024 JP 1998-504196 19970626  
 AT 224884 E 20021015 AT 1997-931281 19970626  
 ES 2179353 T3 20030116 ES 1997-931281 19970626  
 KR 2000022380 A 20000425 KR 1998-710811 19981230  
 PRIORITY APPLN. INFO.: US 1996-674391 A 19960701  
 WO 1997-US10696 W 19970626  
 OTHER SOURCE(S): MARPAT 128:114963  
 GI

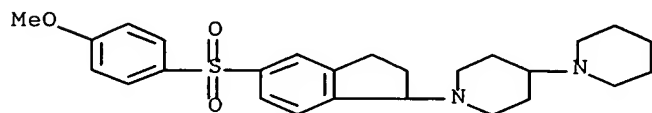


AB Title compds. [I; R<sup>1</sup>, R<sup>2</sup> = H, alk(en)yl, phenylalkyl, etc.; R<sup>3</sup> = (un)substituted piperidino or -piperazino; R<sup>4</sup> = H or 1 or 2 of halo, alkyl, alkoxy, Ph, etc.; R<sup>5</sup> = ZR; R = (un)substituted Ph or -heteroaryl; Z = O, CO, SOO-2, etc.; Z<sup>1</sup> = O, SOO-2, CH<sub>2</sub>; Z<sup>2</sup> = bond or (CH<sub>2</sub>)<sub>1-3</sub>] were prepared. Thus, 5-fluoroindanone was condensed with PhSO<sub>2</sub>Na and the reduced product aminated by N-hydroxyethylpiperazine to give title compound II. Data for biol. activity of I were given.

IT **201745-57-5P 201745-59-7P 201745-61-1P 201745-64-4P**  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of piperazine and piperidine derivs. as muscarinic antagonists)

RN 201745-57-5 HCAPLUS

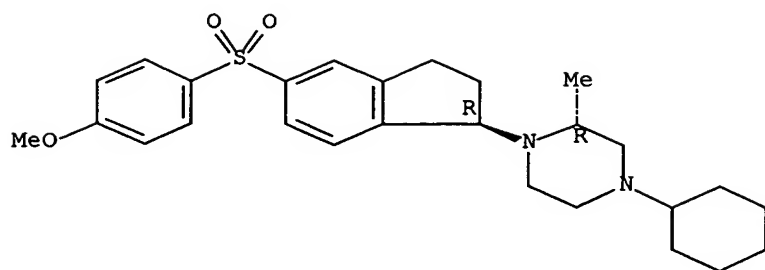
CN 1,4'-Bipiperidine, 1'-[2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]- (9CI) (CA INDEX NAME)



RN 201745-59-7 HCAPLUS

CN Piperazine, 4-cyclohexyl-1-[(1R)-2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]-2-methyl-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

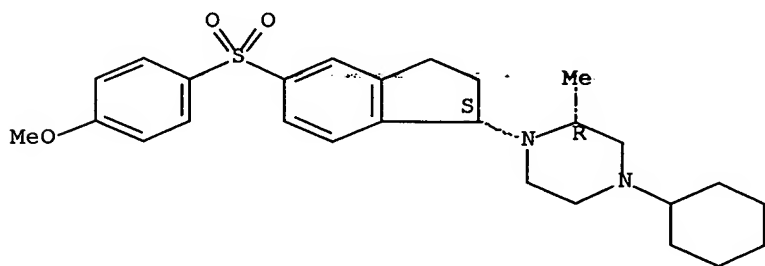


● HCl

RN 201745-61-1 HCAPLUS

CN Piperazine, 4-cyclohexyl-1-[(1S)-2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]-2-methyl-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

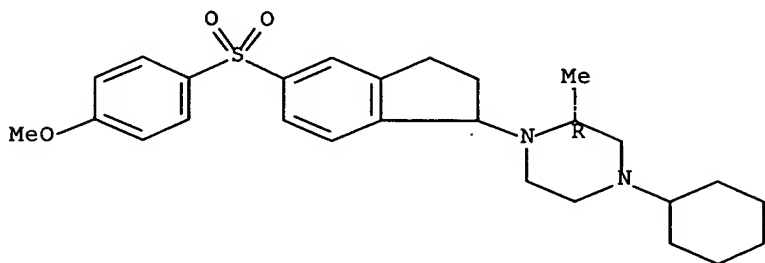


● HCl

RN 201745-64-4 HCAPLUS

CN Piperazine, 4-cyclohexyl-1-[2,3-dihydro-5-[(4-methoxyphenyl)sulfonyl]-1H-inden-1-yl]-2-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



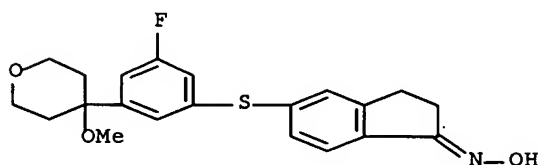
REFERENCE COUNT:

9

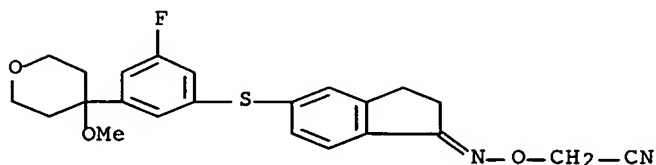
THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

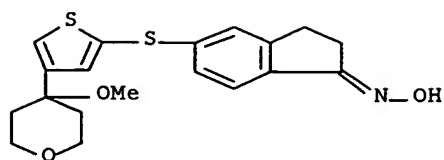
ACCESSION NUMBER: 1996:108631 HCAPLUS Full-text  
 DOCUMENT NUMBER: 124:288419  
 TITLE: Oximes: a new class of methoxytetrahydropyranyl inhibitors of leukotriene biosynthesis with high in vitro and in vivo potency  
 AUTHOR(S): Ple, Patrick A.; Bird, T. Geoffrey C.  
 CORPORATE SOURCE: Zeneca Pharma, Centre Recherches, Reims, 51064, Fr.  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(2), 127-32  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Work aimed at further improving the in vivo activity of methoxytetrahydropyranyl inhibitors of leukotriene biosynthesis has led to the discovery of a series of oximes, members of which are more potent in vivo than ZD2138.  
 IT **175437-43-1 175437-44-2 175437-45-3 175437-46-4 175437-57-7 175437-59-9**  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (high in vitro and in vivo potency methoxytetrahydropyranyl oxime inhibitors of leukotriene biosynthesis)  
 RN 175437-43-1 HCAPLUS  
 CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-2,3-dihydro-, oxime (9CI) (CA INDEX NAME)



RN 175437-44-2 HCAPLUS  
 CN Acetonitrile, [[[5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-2,3-dihydro-1H-inden-1-ylidene]amino]oxy]- (9CI) (CA INDEX NAME)

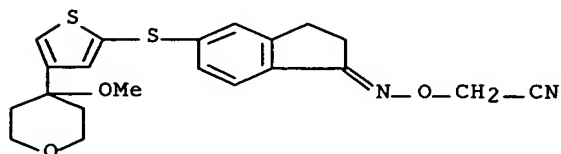


RN 175437-45-3 HCAPLUS  
 CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2H-pyran-4-yl)-2-thienyl]thio]-, oxime (9CI) (CA INDEX NAME)



RN 175437-46-4 HCAPLUS

CN Acetonitrile, [[[2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2H-pyran-4-yl)-2-thienyl]thio]-1H-inden-1-ylidene]amino]oxy]- (9CI) (CA INDEX NAME)

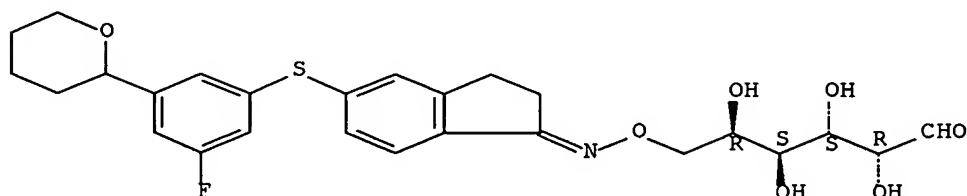


RN 175437-57-7 HCAPLUS

CN D-Galactose, 6-O-[[5-[[3-fluoro-5-(tetrahydro-2H-pyran-2-yl)phenyl]thio]-2,3-dihydro-1H-inden-1-ylidene]amino]- (9CI) (CA INDEX NAME)

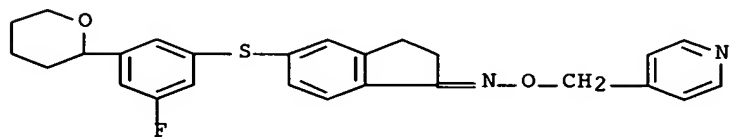
Absolute stereochemistry.

Double bond geometry unknown.



RN 175437-59-9 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-2H-pyran-2-yl)phenyl]thio]-2,3-dihydro-, O-(4-pyridinylmethyl)oxime (9CI) (CA INDEX NAME)



L21 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:529163 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 123:44332

TITLE: High-sensitivity positively charging  
electrophotographic photoreceptor

INVENTOR(S): Ooshiba, Tomomi; Hirose, Hisahiro; Hai, Genko;

PATENT ASSIGNEE(S): Fujimoto, Shingo  
 SOURCE: Konishiroku Photo Ind, Japan  
 Jpn. Kokai Tokkyo Koho, 44 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07056369	A2	19950303	JP 1993-199586	19930811
PRIORITY APPLN. INFO.:			JP 1993-199586	19930811

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

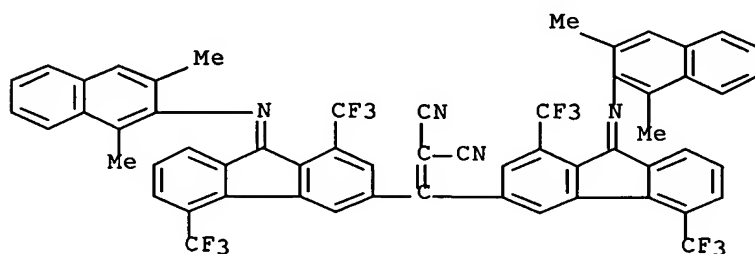
AB The photoreceptor has an elec. conductive support coated with a photosensitive layer containing (heterocyclic) aromatic compound I, II, III, or IV [Q, Q1-3 = O, C(CN)2, CHCN, CY2, C(CO2R)2, CHCO2R, CHR, NR, HCN; Y = halo; R = H, alkyl, Ph, heterocyclic group; X = O, CO, NH, (substituted) aliphatic group, aromatic hydrocarbyl; R, R1-3 = (substituted) alkyl, aryl, alkoxy, acyl, ester, cyano, NO2, amide, sulfone, sulfonamide, OH, CHO, halo; A1-2, B1-2 = (substituted) aromatic hydrocarbyl, heterocyclic group; l, m, j, k ≥ 0] as charge-transporting agents. The photoreceptor showed low residual potential and gave clear images.

IT 163967-54-2

RL: DEV (Device component use); USES (Uses)  
 (electrophotog. photoreceptor containing (heterocyclic) aromatic compound charge-transporting agent with high sensitivity)

RN 163967-54-2 HCAPLUS

CN Propanedinitrile, [bis[9-[(1,3-dimethyl-2-naphthalenyl)imino]-1,5-bis(trifluoromethyl)-9H-fluoren-3-yl]methylene]- (9CI) (CA INDEX NAME)



L21 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:70 HCAPLUS Full-text

DOCUMENT NUMBER: 122:187392

TITLE: Preparation of [heterocyclarylthio]aryl ketoximes  
 and analogs as 5-lipoxygenase inhibitors

INVENTOR(S): Bird, Thomas Geoffrey Colerick; Ple, Patrick

PATENT ASSIGNEE(S): Zeneca Ltd., UK; Zeneca-Pharma

SOURCE: Eur. Pat. Appl., 85 pp.

CODEN: EPXXDW



DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 555068	A1	19930811	EP 1993-300782	19930203
EP 555068	B1	19960410		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
ZA 9300504	A	19930809	ZA 1993-504	19930122
AU 9331972	A1	19930812	AU 1993-31972	19930122
AU 658964	B2	19950504		
HU 63840	A2	19931028	HU 1993-272	19930203
AT 136546	E	19960415	AT 1993-300782	19930203
ES 2086878	T3	19960701	ES 1993-300782	19930203
CA 2088864	AA	19930808	CA 1993-2088864	19930205
NO 9300411	A	19930809	NO 1993-411	19930205
JP 05286957	A2	19931102	JP 1993-18574	19930205
US 5332757	A	19940726	US 1993-14564	19930208
US 5482966	A	19960109	US 1994-240464	19940613
PRIORITY APPLN. INFO.:			EP 1992-400318	A 19920207
			EP 1992-402764	A 19921009
			US 1993-14564	A3 19930208

OTHER SOURCE(S): MARPAT 122:187392

AB R5ON:CR4Z1AXZ2C(OR1)R2R3 [A = bond, alkylene; R1 = alk(en)yl; R2R3 = atoms to complete a heterocyclic ring; R4 = H, alkyl, Ph, etc.; R5 = H, alk(en)yl, alkanoyl, CONH2, etc.; X = O, SO0-2; Z1 = phenylene, heteroarylene, etc.; Z2 = phenylene, pyridinediyl, thiophenediyl, etc.] were prepared Thus, 4-(2-methyl-1,3-dioxolan-2-yl)benzenethiol (preparation in 4 steps from 4-BrC6H4COME given) was condensed with (2S,4R)-4-(3,5-difluorophenyl)-4-methoxy-2-methyltetrahydropyran and the product converted in 2 steps to title compound (2S,4R)-I which had ID50 of .apprx.0.05mg/kg orally against zymosan-induced LTB4 production in rat subcutaneous air pouch.

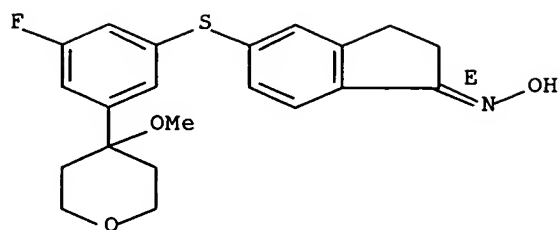
IT 158346-94-2P 158346-95-3P 158346-96-4P  
 158346-97-5P 158346-98-6P 161384-62-9P  
 161385-07-5P 161385-11-1P 161385-14-4P  
 161385-17-7P 161385-36-0P 161385-37-1P  
 161385-53-1P 161385-54-2P 161385-55-3P  
 161385-56-4P 161385-67-7P 161385-68-8P  
 161385-75-7P 161385-78-0P 161509-87-1P  
 161509-88-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of [(heterocyclyl)arylthio]aryl ketoximes and analogs as 5-lipoxygenase inhibitors)

RN 158346-94-2 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-2,3-dihydro-, oxime, (E)- (9CI) (CA INDEX NAME)

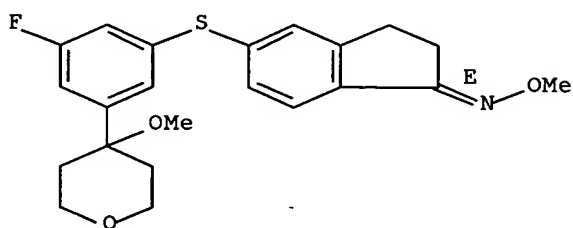
Double bond geometry as shown.



RN 158346-95-3 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-2,3-dihydro-, O-methyloxime, (E)- (9CI) (CA INDEX NAME)

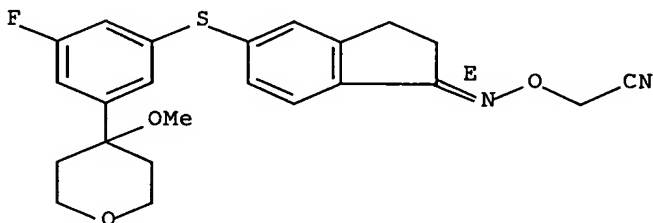
Double bond geometry as shown.



RN 158346-96-4 HCAPLUS

CN Acetonitrile, [[5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-2,3-dihydro-1H-inden-1-ylidene]amino]oxy]-, (E)- (9CI) (CA INDEX NAME)

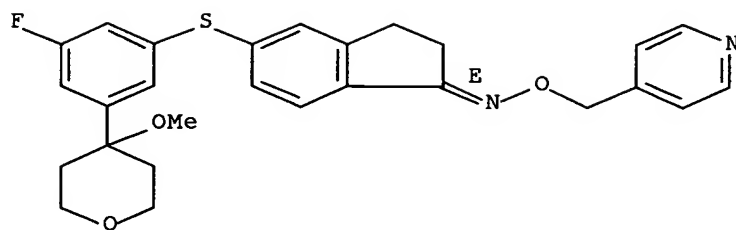
Double bond geometry as shown.



RN 158346-97-5 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-2,3-dihydro-, O-(4-pyridinylmethyl)oxime, (E)- (9CI) (CA INDEX NAME)

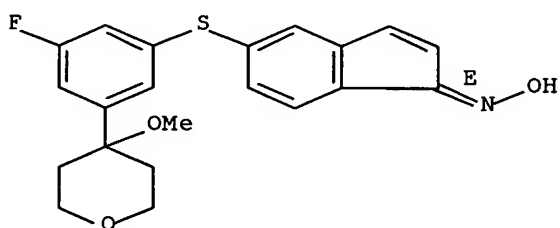
Double bond geometry as shown.



RN 158346-98-6 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-, oxime, (E)- (9CI) (CA INDEX NAME)

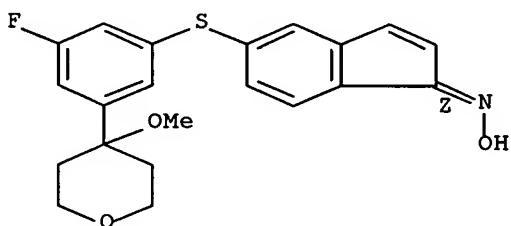
Double bond geometry as shown.



RN 161384-62-9 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-, oxime, (Z)- (9CI) (CA INDEX NAME)

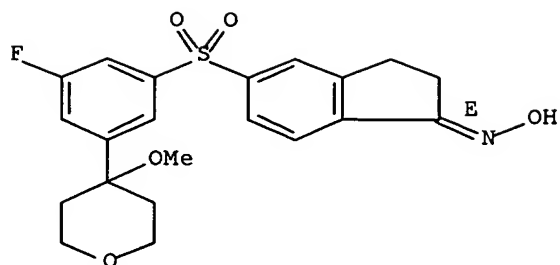
Double bond geometry as shown.



RN 161385-07-5 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]sulfonyl]-2,3-dihydro-, oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

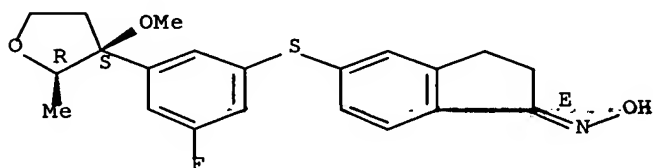


RN 161385-11-1 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-3-methoxy-2-methyl-3-furanyl)phenyl]thio]-2,3-dihydro-, oxime, [2 $\alpha$ ,3 $\alpha$ ,3(E)]- (9CI)  
(CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

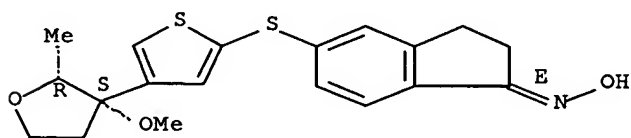


RN 161385-14-4 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-3-methoxy-2-methyl-3-furanyl)-2-thienyl]thio]-, oxime, [2 $\alpha$ ,3 $\alpha$ ,3(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

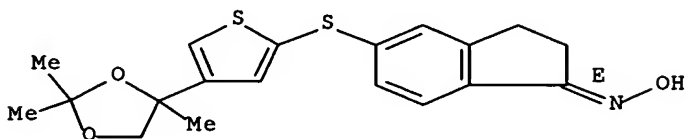
Double bond geometry as shown.



RN 161385-17-7 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(2,2,4-trimethyl-1,3-dioxolan-4-yl)-2-thienyl]thio]-, oxime, (E)- (9CI) (CA INDEX NAME)

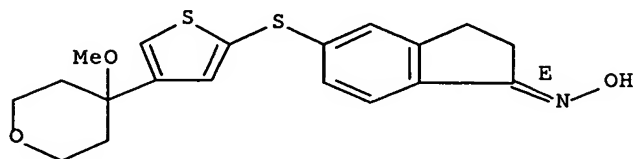
Double bond geometry as shown.



RN 161385-36-0 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2H-pyran-4-yl)-2-thienyl]thio]-, oxime, (E)- (9CI) (CA INDEX NAME)

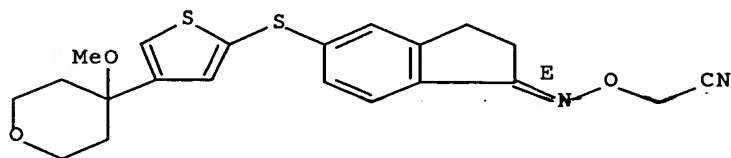
Double bond geometry as shown.



RN 161385-37-1 HCAPLUS

CN Acetonitrile, [[[2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2H-pyran-4-yl)-2-thienyl]thio]-1H-inden-1-ylidene]amino]oxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

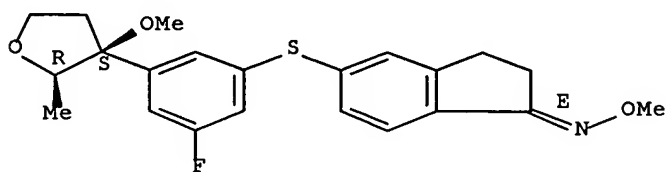


RN 161385-53-1 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-3-methoxy-2-methyl-3-furanyl)phenyl]thio]-2,3-dihydro-, O-methyloxime, [2 $\alpha$ ,3 $\alpha$ ,3(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

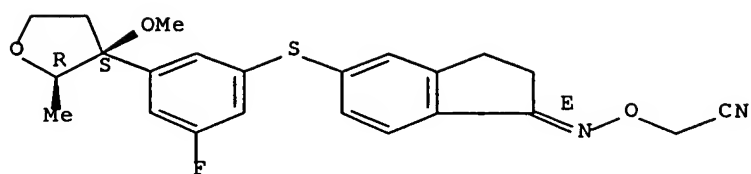


RN 161385-54-2 HCAPLUS

CN Acetonitrile, [[[[5-[[3-fluoro-5-(tetrahydro-3-methoxy-2-methyl-3-furanyl)phenyl]thio]-2,3-dihydro-1H-inden-1-ylidene]amino]oxy]-, [2 $\alpha$ ,3 $\alpha$ ,3(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

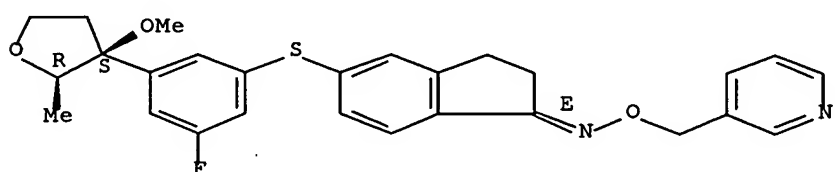


RN 161385-55-3 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-3-methoxy-2-methyl-3-furanyl)phenyl]thio]-2,3-dihydro-, O-(3-pyridinylmethyl)oxime, [2 $\alpha$ ,3 $\alpha$ ,3(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

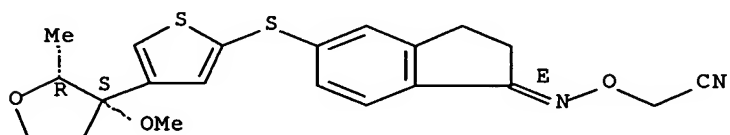


RN 161385-56-4 HCAPLUS

CN Acetonitrile, [[[2,3-dihydro-5-[[4-(tetrahydro-3-methoxy-2-methyl-3-furanyl)-2-thienyl]thio]-1H-inden-1-ylidene]amino]oxy]-, [2 $\alpha$ ,3 $\alpha$ ,3(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

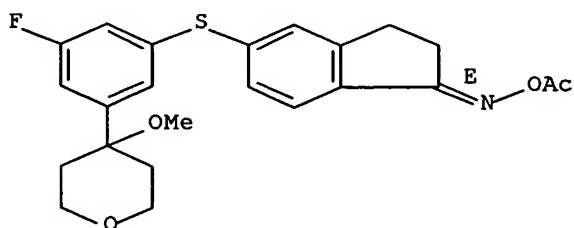
Double bond geometry as shown.



RN 161385-67-7 HCAPLUS

CN 1H-Inden-1-one, 5-[[3-fluoro-5-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]thio]-2,3-dihydro-, O-acetyloxime, (E)- (9CI) (CA INDEX NAME)

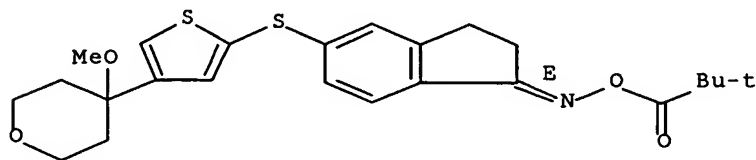
Double bond geometry as shown.



RN 161385-68-8 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2H-pyran-4-yl)-2-thienyl]thio]-, O-(2,2-dimethyl-1-oxopropyl)oxime, (E)- (9CI) (CA INDEX NAME)

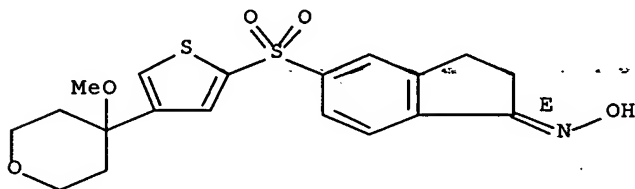
Double bond geometry as shown.



RN 161385-75-7 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2H-pyran-4-yl)-2-thienyl]sulfonyl]-, oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

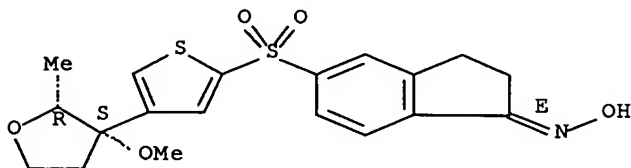


RN 161385-78-0 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-3-methoxy-2-methyl-3-furanyl)-2-thienyl]sulfonyl]-, oxime, [2 $\alpha$ ,3 $\alpha$ ,3(E)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

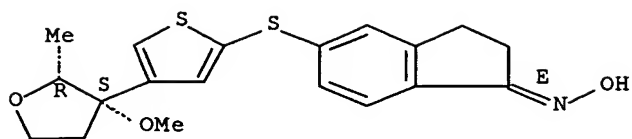


RN 161509-87-1 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-3-methoxy-2-methyl-3-furanyl)-2-thienyl]thio]-, oxime, [2R-[2 $\alpha$ ,3 $\alpha$ ,3(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

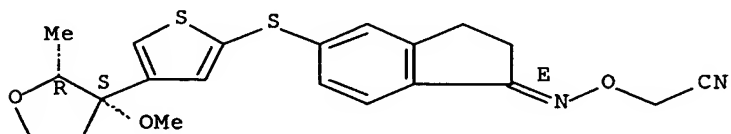


RN 161509-88-2 HCAPLUS

CN Acetonitrile, [[2,3-dihydro-5-[[4-(tetrahydro-3-methoxy-2-methyl-3-furanyl)-2-thienyl]thio]-1H-inden-1-ylidene]amino]oxy]-, [2R-[2 $\alpha$ ,3 $\alpha$ ,3(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 161386-96-5P 161387-21-9P

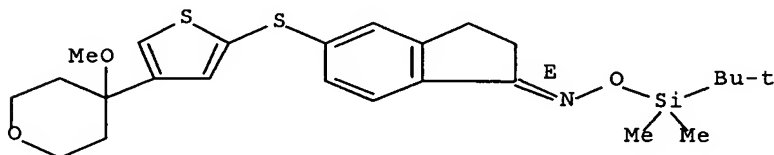
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [(heterocyclyl)arylthio]aryl ketoximes and analogs as 5-lipoxygenase inhibitors)

RN 161386-96-5 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2H-pyran-4-yl)-2-thienyl]thio]-, O-[(1,1-dimethylethyl)dimethylsilyl]oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



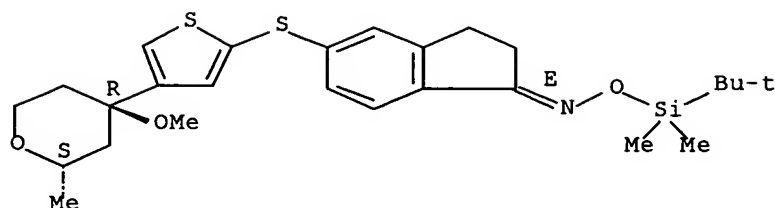
RN 161387-21-9 HCAPLUS

CN 1H-Inden-1-one, 2,3-dihydro-5-[[4-(tetrahydro-4-methoxy-2-methyl-2H-pyran-4-yl)-2-thienyl]thio]-, O-[(1,1-dimethylethyl)dimethylsilyl]oxime, [2S-[2 $\alpha$ ,4 $\beta$ ,4(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

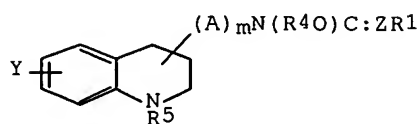




L21 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1994:457344 HCAPLUS Full-text  
 DOCUMENT NUMBER: 121:57344  
 TITLE: Preparation of antiinflammatory N-(substituted tetrahydroquinolinyl)hydroxamic acids and N-hydroxy-N-(substituted tetrahydroquinolinyl)ureas  
 INVENTOR(S): Stevens, Rodney W.; Ikeda, Takafumi; Wakabayashi, Hiroaki; Nakane, Masami  
 PATENT ASSIGNEE(S): Pfizer Inc., USA  
 SOURCE: U.S., 25 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5256789	A	19931026	US 1992-835934	19920218
PRIORITY APPLN. INFO.:			US 1992-835934	19920218
OTHER SOURCE(S):	MARPAT 121:57344			

GI



I

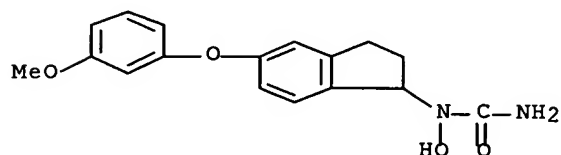
AB Title compds. I (R1 = C1-4 alkyl, R3R2N wherein R2, R3 = H, C1-4 alkyl; R4 = H, a pharmaceutically acceptable cation, aroyl, C1-12 alkanoyl; R5 = H, C1-6 alkyl, C3-6 alkenyl, C1-6 alkanoyl, aryl, arylalkyl, aroyl; m = 0,1; A = C1-6 alkylene, C2-6 alkenylene, C2-6 alkylidene; Y = H, halo, HO, NC, C1-12 alkyl haloalkyl, aminocarbonyl, etc.; Z = O, S), useful as lipoxygenase inhibitors and thus as antiinflammatories (no data), are prepared To a mixture of 1-benzyl-1,2,3,4-tetrahydroquinolin-6-ylethan-1-ol, BocNH-OBoc, and Ph3P in MePh was added di-Et azodicarboxylate to give the hydroxyazine derivative to which in CH2Cl2 was added CF3CO2H to give I (R1 = H2N, R4 = Y = H, R5 = PhCH2, m = 1, A = CH2CH2, Z = O). Addnl. title compds. were prepared

IT 138910-85-7P 138910-87-9P 138910-90-4P  
 138910-91-5P 138910-92-6P 138910-93-7P  
 138910-94-8P 138910-97-1P 138911-01-0P  
 138911-05-4P 138911-06-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

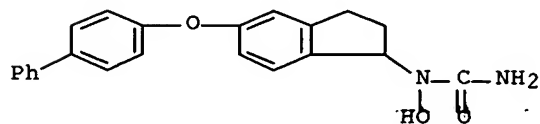
(preparation and reaction of, in preparation of antiinflammatories)

RN 138910-85-7 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(3-methoxyphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)

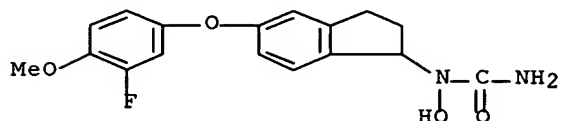
RN 138910-87-9 HCAPLUS

CN Urea, N-[5-([1,1'-biphenyl]-4-yloxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy- (9CI) (CA INDEX NAME)



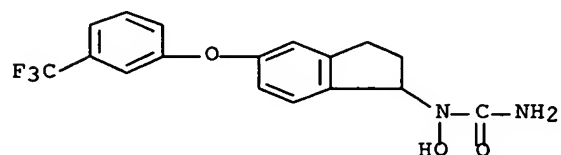
RN 138910-90-4 HCAPLUS

CN Urea, N-[5-(3-fluoro-4-methoxyphenoxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy- (9CI) (CA INDEX NAME)



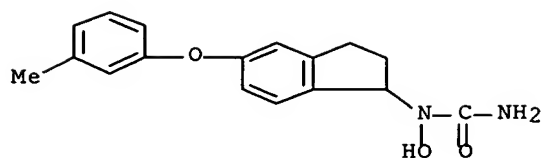
RN 138910-91-5 HCAPLUS

CN Urea, N-[2,3-dihydro-5-[3-(trifluoromethyl)phenoxy]-1H-inden-1-yl]-N-hydroxy- (9CI) (CA INDEX NAME)



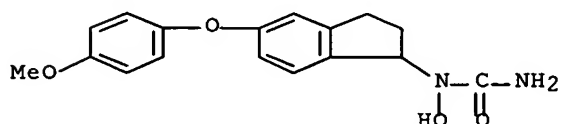
RN 138910-92-6 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(3-methylphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



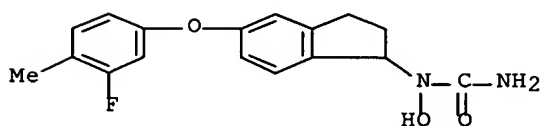
RN 138910-93-7 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(4-methoxyphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



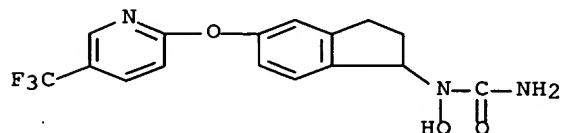
RN 138910-94-8 HCAPLUS

CN Urea, N-[5-(3-fluoro-4-methylphenoxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



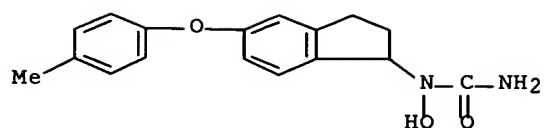
RN 138910-97-1 HCAPLUS

CN Urea, N-[2,3-dihydro-5-[[5-(trifluoromethyl)-2-pyridinyl]oxy]-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



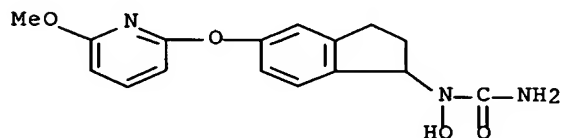
RN 138911-01-0 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(4-methylphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



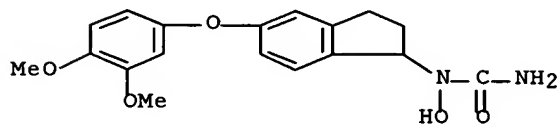
RN 138911-05-4 HCAPLUS

CN Urea, N-[2,3-dihydro-5-[(6-methoxy-2-pyridinyl)oxy]-1H-inden-1-yl]-N-hydroxy- (9CI) (CA INDEX NAME)



RN 138911-06-5 HCAPLUS

CN Urea, N-[5-(3,4-dimethoxyphenoxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy- (9CI) (CA INDEX NAME)



L21 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:83558 HCAPLUS Full-text

DOCUMENT NUMBER: 116:83558

TITLE: Preparation of N-hydroxy-N-(quinolinylalkyl)ureas and analogs as lipoxygenase inhibitors

INVENTOR(S): Stevens, Rodney William; Ikeda, Takafumi; Wakabayashi, Hiroaki; Nakane, Masami

PATENT ASSIGNEE(S): Pfizer Inc., Japan

SOURCE: PCT Int. Appl., 81 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

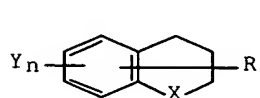
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

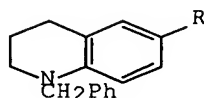
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9116298	A1	19911031	WO 1991-US2674	19910418
W: AU, BR, CA, FI, HU, KR, NO, PL, SU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, NL, SE				
JP 06065204	A2	19940308	JP 1991-216711	19910301
JP 07005560	B4	19950125		
IL 97866	A1	19971120	IL 1991-97866	19910416
CA 2078216	AA	19911021	CA 1991-2078216	19910418

AU 9177986	A1	19911111	AU 1991-77986	19910418
AU 646865	B2	19940310		
EP 525111	A1	19930203	EP 1991-909090	19910418
EP 525111	B1	19950614		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 61723	A2	19930301	HU 1992-3286	19910418
BR 9106367	A	19930427	BR 1991-6367	19910418
PL 165843	B1	19950228	PL 1991-296500	19910418
ES 2073755	T3	19950816	ES 1991-909090	19910418
RU 2108324	C1	19980410	RU 1992-16453	19910418
CN 1060286	A	19920415	CN 1991-103231	19910419
CN 1033325	B	19961120		
ZA 9102935	A	19921125	ZA 1991-2935	19910419
NO 9204045	A	19921019	NO 1992-4045	19921019
NO 180482	B	19970120		
NO 180482	C	19970430		
PRIORITY APPLN. INFO.:			JP 1990-105048	A 19900420
			WO 1991-US2674	A 19910418
OTHER SOURCE(S):			MARPAT 116:83558	
GI				



I



II

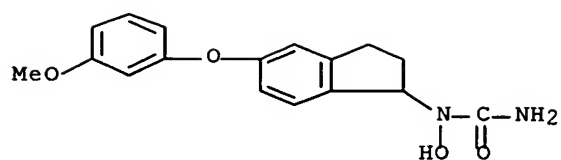
AB Title compds. [I; R = AmN(OR<sub>4</sub>)C(:Z)R<sub>1</sub>; A = alkylene, alkenylene, alkylidene; R<sub>1</sub> = H, (alkoxy)alkyl, alkenyl, alkylthioalkyl, NR<sub>2</sub>R<sub>3</sub>; R<sub>2</sub>, R<sub>3</sub> = H, alkyl, OH, (un)substituted aryl; R<sub>4</sub> = H, alkanoyl, aroyl, pharmaceutically acceptable cation; X = bond, O, S, (substituted) imino; Y = H, halo, OH, cyano, (halo)alkyl, etc.; Z = O, S; m = 0, 1; n = 1-3] were prepared. Thus, tetrahydroquinolinylethanol II (R = CH<sub>2</sub>CH<sub>2</sub>OH) was condensed with BocNHOBoc and the deprotected product condensed with Me<sub>3</sub>SiNCO to give, after hydrolysis, [R = CH<sub>2</sub>CH<sub>2</sub>N(OH)CONH<sub>2</sub>]. I had IC<sub>50</sub> of 0.1 to 30  $\mu$ M against lipoxigenase.

IT 138910-85-7P 138910-87-9P 138910-90-4P  
138910-91-5P 138910-92-6P 138910-93-7P  
138910-94-8P 138910-97-1P 138911-01-0P  
138911-05-4P 138911-06-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as lipoxigenase inhibitor)

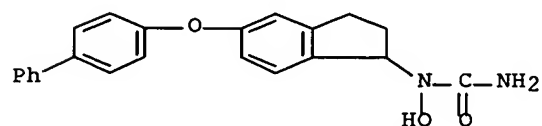
RN 138910-85-7 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(3-methoxyphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



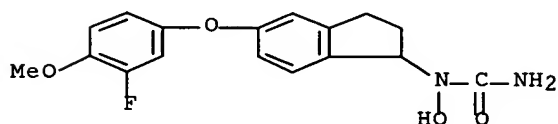
RN 138910-87-9 HCAPLUS

CN Urea, N-[5-([1,1'-biphenyl]-4-yloxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy-  
(9CI) (CA INDEX NAME)



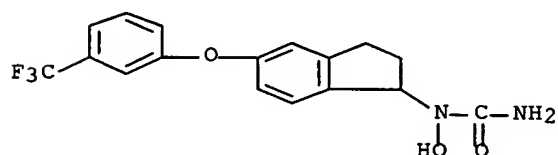
RN 138910-90-4 HCAPLUS

CN Urea, N-[5-(3-fluoro-4-methoxyphenoxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy-  
(9CI) (CA INDEX NAME)



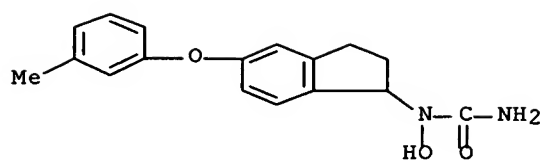
RN 138910-91-5 HCAPLUS

CN Urea, N-[2,3-dihydro-5-[3-(trifluoromethyl)phenoxy]-1H-inden-1-yl]-N-hydroxy-  
(9CI) (CA INDEX NAME)



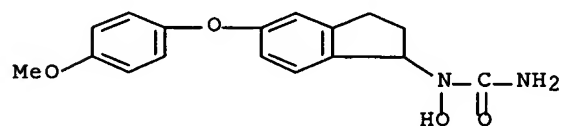
RN 138910-92-6 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(3-methylphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



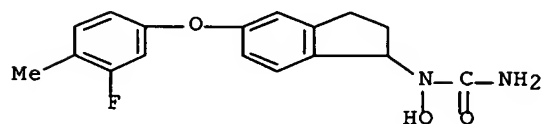
RN 138910-93-7 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(4-methoxyphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



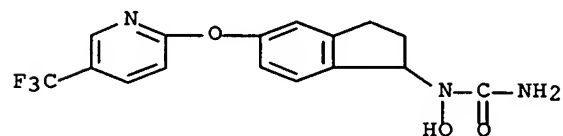
RN 138910-94-8 HCAPLUS

CN Urea, N-[5-(3-fluoro-4-methylphenoxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



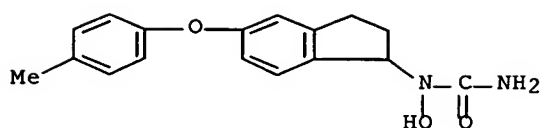
RN 138910-97-1 HCAPLUS

CN Urea, N-[2,3-dihydro-5-[[5-(trifluoromethyl)-2-pyridinyl]oxy]-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



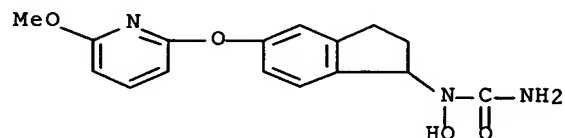
RN 138911-01-0 HCAPLUS

CN Urea, N-[2,3-dihydro-5-(4-methylphenoxy)-1H-inden-1-yl]-N-hydroxy- (9CI)  
(CA INDEX NAME)



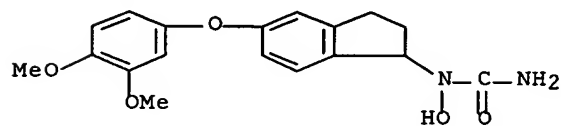
RN 138911-05-4 HCAPLUS

CN Urea, N-[2,3-dihydro-5-[(6-methoxy-2-pyridinyl)oxy]-1H-inden-1-yl]-N-hydroxy- (9CI) (CA INDEX NAME)



RN 138911-06-5 HCAPLUS

CN Urea, N-[5-(3,4-dimethoxyphenoxy)-2,3-dihydro-1H-inden-1-yl]-N-hydroxy- (9CI) (CA INDEX NAME)



=> => => d stat que 123 nos

L1 STR  
 L2 3144 SEA FILE=REGISTRY SSS FUL L1  
 L3 STR  
 L4 207 SEA FILE=REGISTRY SUB=L2 SSS FUL L3  
 L15 STR  
 L17 2 SEA FILE=REGISTRY SUB=L4 SSS FUL L15  
 L18 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L17  
 L19 205 SEA FILE=REGISTRY ABB=ON PLU=ON L4 NOT L17  
 L20 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L19  
 L21 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 NOT L18  
 L22 24 SEA FILE=HCAPLUS ABB=ON PLU=ON "TONG LING"/AU  
 L23 23 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 NOT (L18 OR L21)

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L23 ANSWER 1 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:980797 HCAPLUS Full-text

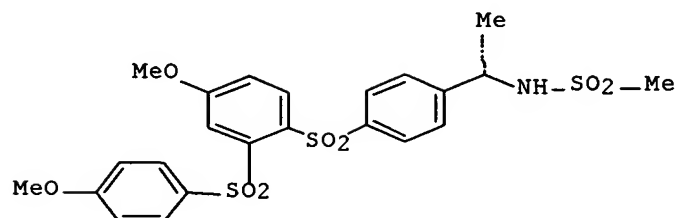
DOCUMENT NUMBER: 143:318371

TITLE: Triaryl bis-sulfones as cannabinoid-2 receptor ligands: SAR studies

AUTHOR(S): Shankar, Bandarpalle B.; Lavey, Brian J.; Zhou,



Guowei; Spitler, James A.; **Tong, Ling**;  
 Rizvi, Razia; Yang, De-Yi; Wolin, Ronald; Kozlowski,  
 Joseph A.; Shih, Neng-Yang; Wu, Jie; Hipkin, R.  
 William; Gonsiorek, Waldemar; Lunn, Charles A.  
 CORPORATE SOURCE: Department of Chemistry, Schering-Plough Research  
 Institute, Kenilworth, NJ, 07033-0539, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),  
 15(20), 4417-4420  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The authors recently reported that compound (I) is a potent inhibitor of the  
 CB2 receptor with high selectivity over CB1. This paper describes the SAR  
 development for this class of compds. Variation of the substitution pattern  
 on the aromatic rings, as well as the groups linking them together, led to  
 sub-nanomolar inhibitors of the CB2 receptor, with high selectivity over CB1.  
 REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:812566 HCAPLUS Full-text  
 TITLE: Configuration, conformation and crystal structure of  
 rabdosiainin b  
 AUTHOR(S): Li, Bao Lin; Pan, Yuan Jiang; Li, Jin; **Tong**,  
**Ling**; Yu, Kai Bei  
 CORPORATE SOURCE: School of Chemistry and Material Science, Shaanxi  
 Normal University, Shaanxi, 710062, Peop. Rep. China  
 SOURCE: Crystal Research and Technology (2005), 40(8), 810-814  
 CODEN: CRTEDF; ISSN: 0232-1300  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Rabdosiainin B, 7,20-epoxy-7 $\beta$ -hydroxy-1 $\alpha$ ,6 $\beta$ ,11 $\alpha$ ,15-be ta.-tetraacetoxy-ent-  
 kaur-16-ene, C<sub>28</sub>H<sub>38</sub>O<sub>10</sub>, was the first isolated from *Isodon henryi*. It  
 consists of three six-membered rings A, B, C and one five-membered ring D.  
 The fused-ring system A, B and C are in chair, boat and chair conformations,  
 resp., and ring D is in an envelope conformation, on the basis of NMR and X-  
 ray diffraction anal. The crystal of rabdosiainin B is in orthorhombic crystal  
 system with space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, lattice consts.: a=9.969(1)Å, b=15.400(3)Å,  
 and c= 17.624(3)Å, Z=4.  
 REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 3 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:705198 HCAPLUS Full-textTITLE: Tyrosine hydroxylase in rat auditory midbrain:  
Distribution and changes following deafnessAUTHOR(S): **Tong, Ling**; Altschuler, Richard A.; Genene  
Holt, AvrilCORPORATE SOURCE: Kresge Hearing Research Institute, Department of  
Otolaryngology/Head Neck Surgery, University of  
Michigan, Ann Arbor, MI, 48109, USASOURCE: Hearing Research (2005), 206(1-2), 28-41  
CODEN: HERED3; ISSN: 0378-5955

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tyrosine hydroxylase (TH), a key enzyme in the catecholaminergic pathway, allows for the differentiation of dopaminergic neurons. We previously showed decreases in TH gene expression in the rat inferior colliculus (IC) 3 and 21 days following deafness. In the present study, we characterized the normal distribution of TH as well as changes following deafness (bilateral cochlear ablation) in the IC and nuclei of the lateral lemniscus. Immunostaining was compared in three groups of rats: normal hearing (n = 8), 21 day deaf (n = 5) and 90 days following deafening (n = 5). Many TH immunoreactive fibers and puncta were identified in the IC and nuclei of the lateral lemniscus of normal hearing animals and labeling was most dense in the external cortex of the IC. We also identified immunolabeling for fibers and puncta for another catecholaminergic enzyme, dopamine  $\beta$  hydroxylase (DBH), but not phenylethanolamine-N- methyltransferase (PNMT). Neurons immunopos. for TH but not DBH or PNMT were observed in the dorsal cortex and dorsal horn of the central nucleus of the IC and ventral and intermediate lemniscus. In the central nucleus of the IC and dorsal lateral lemniscus many lightly labeled TH neurons were also DBH pos. Although the number of immunopos. cells in the IC and lemniscus declined 3 wk and 3 mo after deafening, the decline was not significant at three weeks in the VNLL nor after three months in the dorsal cortex. Immunolabeling for TH decreased significantly in IC and lemniscus 3 wk and 3 mo following deafening. These results suggest a role for dopaminergic neurons and fibers in deafness-related plasticity.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 4 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:674582 HCAPLUS Full-text

DOCUMENT NUMBER: 143:311869

TITLE: Improving nonthrombogenicity of chitin with  
zwitterionic structure of sulfobetaineAUTHOR(S): Zhu, Jun; Pan, Chang-wang; **Tong, Ling**; Yan,  
Han; Shen, Jian; Lin, Si-congCORPORATE SOURCE: Research Center of Surface & Interface Chemistry and  
Engineering Technology, Nanjing University, Nanjing,  
210093, Peop. Rep. ChinaSOURCE: Chinese Journal of Polymer Science (2005), 23(4),  
449-452

CODEN: CJPSEG; ISSN: 0256-7679

PUBLISHER: World Scientific Publishing Co. Pte. Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In order to improve the nonthrombogenicity of chitin, a new monomer, N,N-dimethyl( $\beta$ -hydroxyethyloxyethyl) ammonium propanesulfonate (DHAPS) was designed, synthesized and grafted onto the chitin membrane by using hexamethylene diisocyanate (HDI) as a coupling agent. Surface anal. of the

grafted membranes by ATR-FTIR and XPS confirmed that DHAPS has been successfully grafted onto the membrane surface. The platelet resistant property of the grafted membranes was evaluated by a platelet-rich plasma adhesion method. The results showed that platelet-adhesive resistance of the modified membrane has been greatly improved.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 5 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:502409 HCAPLUS Full-text

DOCUMENT NUMBER: 143:167454

TITLE: Deafness-related plasticity in the inferior colliculus: Gene expression profiling following removal of peripheral activity

AUTHOR(S): Holt, Avril Genene; Asako, Mikiya; Lomax, Catherine A.; MacDonald, James W.; Tong, Ling; Lomax, Margaret I.; Altschuler, Richard A.

CORPORATE SOURCE: Kresge Hearing Research Institute, Department of Otolaryngology/Head Neck Surgery, University of Michigan, Ann Arbor, MI, USA

SOURCE: Journal of Neurochemistry (2005), 93(5), 1069-1086  
CODEN: JONRA9; ISSN: 0022-3042

PUBLISHER: Blackwell Publishing Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The inferior colliculus (IC) is a major center of integration in the ascending as well as descending auditory pathways, where both excitatory and inhibitory amino acid neurotransmitters play a key role. When normal input to the auditory system is decreased, the balance between excitation and inhibition in the IC is disturbed. We examined global changes in gene expression in the rat IC 3 and 21 days following bilateral deafening, using Affymetrix GeneChip arrays and focused our anal. on changes in expression of neurotransmission-related genes. Over 1400 probe sets in the Affymetrix Rat Genome U34A Array were identified as genes that were differentially expressed. These genes encoded proteins previously reported to change as a consequence of deafness, such as calbindin, as well as proteins not previously reported to be modulated by deafness, such as clathrin. A subset of 19 differentially expressed genes was further examined using quant. RT-PCR at 3, 21 and 90 days following deafness. These included several GABA, glycine, glutamate receptor and neuropeptide-related genes. Expression of genes for GABA-A receptor subunits  $\beta 2$ ,  $\beta 3$ , and  $\gamma 2$ , plus ionotropic glutamate receptor subunits AMPA 2, AMPA 3, and kainate 2, increased at all three times. Expression of glycine receptor  $\alpha 1$  initially declined and then later increased, while  $\alpha 2$  increased sharply at 21 days. Glycine receptor  $\alpha 3$  increased between 3 and 21 days, but decreased at 90 days. Of the neuropeptide-related genes tested with qRT-PCR, tyrosine hydroxylase decreased approx. 50% at all times tested. Serotonin receptor 2C increased at 3, 21, and 90 days. The 5B serotonin receptor decreased at 3 and 21 days and returned to normal by 90 days. Of the genes tested with qRT-PCR, only glycine receptor  $\alpha 2$  and serotonin receptor 5B returned to normal levels of expression at 90 days. Changes in GABA receptor  $\beta 3$ , GABA receptor  $\gamma 2$ , glutamate receptor 2/3, enkephalin, and tyrosine hydroxylase were further confirmed using immunocytochem.

REFERENCE COUNT: 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 6 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1065070 HCAPLUS Full-text

DOCUMENT NUMBER: 143:247013

TITLE: Calculation of theoretical stages for

liquid-liquid-solid three-phase concurrent flow  
extractor

AUTHOR(S): **Tong, Ling;** Bao, Zonghong; Shi, Meiren  
CORPORATE SOURCE: College of Chemistry and Chemical Engineering, Nanjing  
University of Technology, Nanjing, 210009, Peop. Rep.  
China  
SOURCE: Zhongguo Youzhi (2003), 28(6), 7-11  
CODEN: ZHYOEG; ISSN: 1003-7969  
PUBLISHER: Zhongguo Youzhi Zazhishe  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese

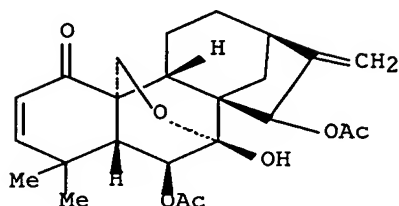
AB A model for calcn. of theor. stages in liquid- liquid-solid three phase leaching was proposed according to the leaching manner of the methanol phase and hexane phase contacting abreast with grounded rapeseed meal. The model correlated the relative flow rate of each material stream entering and leaving the column and the equilibrium solubility of oil in each material stream. The model also included the back mixing effects of the two- phase solvent entrained by the rapeseed marc phase and the average stage efficiency. The model could be used to calculate the theor. stage number of a column in meeting the desired leaching task or to calculate the average stage efficiency for a column in using. The reliability of the model was confirmed by a determination of cascade expts. and the average stage efficiency of cascade expts. was in the range of 0.32-0.54 under different leaching conditions according to the model calcn. The model also indicated that the theor. stages number of a column was influenced slightly by the ratio of methanol to rapeseed (L/kg) and the back mixing amount methanol phase, but obviously by the ratio of hexane to rapeseed (L/kg) and the back mixing amount hexane phase. The model could be applied to provide some useful information and helpful to the design of leachers.

L23 ANSWER 7 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:833060 HCAPLUS Full-text  
DOCUMENT NUMBER: 143:114344  
TITLE: Cocurrent extraction of rapeseed with two-phase  
solvent system  
AUTHOR(S): Bao, Zonghong; **Tong, Ling;** Shi, Meiren  
CORPORATE SOURCE: College of Chemistry and Chemical Engineering, Nanjing  
University of Technology, Nanjing, 210009, Peop. Rep.  
China  
SOURCE: Zhongguo Youzhi (2003), 28(4), 10-14  
CODEN: ZHYOEG; ISSN: 1003-7969  
PUBLISHER: Zhongguo Youzhi Zazhishe  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese

AB To simplify the extraction process for Chinese rapeseed with a two-phase solvent system, consisting of methanol containing 10% water and a small amount of additive as the polar phase and com. hexane as the non-polar phase, a simplified process was proposed by combining two step processing, sep. for the leaching of oil and glucosinolates into one. Cascade expts. were conducted to verify the feasibility of the proposition. The results showed that it was feasible to leach oil and remove glucosinolates simultaneously from Chinese rapeseed within a leaching apparatus Residual oil and glucosinolates in meal could be reduced below 1% and 30  $\mu\text{mol/g}$ , resp., under following conditions: leaching temperature 40-50°, 4 ideal stages, ratio of hexane to rapeseed being 2 (L/kg), ratio of methanol to rapeseed being 5, and water content in methanol phase being 10% (V%). The results of this work could be used for the scaling up of the technique.

L23 ANSWER 8 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:184457 HCAPLUS Full-text  
 DOCUMENT NUMBER: 141:106624  
 TITLE: Stereochemistry structure of odonicin  
 AUTHOR(S): Li, Bao-Lin; Li, Jin; **Tong, Ling**; Pan,  
 Yuan-Jiang; Yu, Kai-Bei  
 CORPORATE SOURCE: School of Chemistry and Material Science, Shaanxi  
 Normal University, Xian, 710062, Peop. Rep. China  
 SOURCE: Bulletin of the Korean Chemical Society (2004), 25(2),  
 304-306  
 CODEN: BKCSDE; ISSN: 0253-2964  
 PUBLISHER: Korean Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



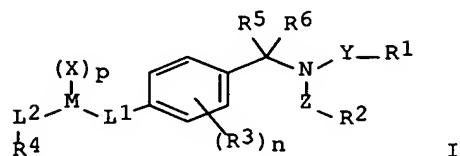
I

AB The stereochem. of an ent-kaurene diterpenoid, odonicin (I), isolated from  
 Isodon henryi, was established on the basis of X-ray diffraction anal.  
 REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 9 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:2853 HCAPLUS Full-text  
 DOCUMENT NUMBER: 140:77029  
 TITLE: Preparation of heteroarene derivatives as cannabinoid  
 receptor agonists  
 INVENTOR(S): Kozlowski, Joseph A.; Shankar, Bandarpalle B.; Shih,  
 Neng-yang; **Tong, Ling**  
 PATENT ASSIGNEE(S): Schering Corporation, USA  
 SOURCE: PCT Int. Appl., 92 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004000807	A1	20031231	WO 2003-US19245	20030617
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,			
	CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU,			
	ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD,			
	MG, MK, MN, MX, MZ, NI, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG,			
	SK, SL, TJ, TM, TN, TR, TT, TZ, UA, US, UZ, VC, VN, YU, ZA, ZM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,			
	KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,			
	FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,			

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 CA 2487346 AA 20031231 CA 2003-2487346 20030617  
 US 2004044051 A1 20040304 US 2003-464174 20030617  
 EP 1539693 A1 20050615 EP 2003-761108 20030617  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 JP 2005533809 T2 20051110 JP 2004-515897 20030617  
 PRIORITY APPLN. INFO.: US 2002-389788P P 20020619  
 WO 2003-US19245 W 20030617  
 OTHER SOURCE(S): MARPAT 140:77029  
 GI



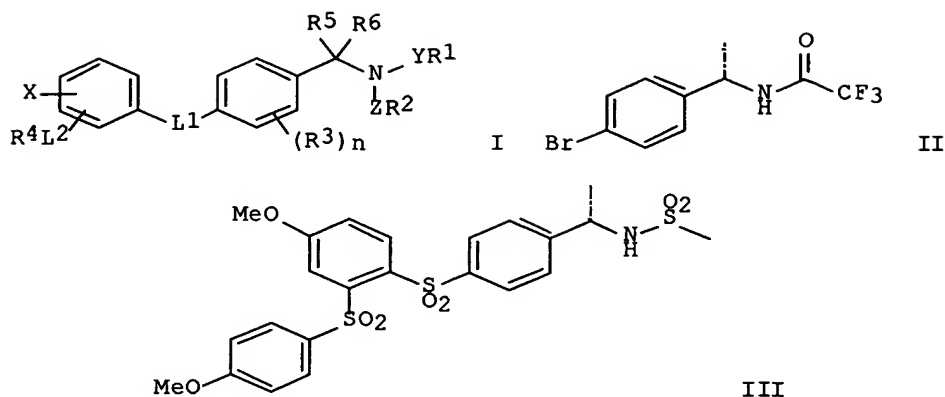
AB Benzylamine and 1-phenylethylamine compds. containing heteroarene such furan, benzofuran, indole, pyridine, and thiofuran of the formula (I) or pharmaceutically acceptable salts thereof [wherein R1, R2 = H, each (un)substituted alkyl, alkenyl, haloalkyl, NH2, cycloalkyl, cycloheteroalkyl, aryl, or heteroaryl; R3 = alkyl, heteroalkyl, aryl, heteroaryl, Br, Cl, F, CF3, OCF2H, OCF3, or alkoxy, wherein R3 can be the same or different and is independently selected when n>1; R4 = (un)substituted H, alkyl, alkenyl, cycloalkyl, cycloheteroalkyl, aryl, or heteroaryl; R5, R6 = H, each (un)substituted alkyl, alkenyl, cycloalkyl, cycloheteroalkyl, aryl, or heteroaryl; R7 = H, each (un)substituted alkyl, alkenyl, haloalkyl, cycloalkyl, cycloheteroalkyl, aryl, or heteroaryl, or two R7 groups can form a ring of 4-7-carbon atoms; L1 = C(R2)2, CO, [CH(OR2)], SO2, SO, S, O, N(R2), CONH, NHCO, CF2, CH:NOR2, CH(NHOR2); L2 = a covalent bond, CH2, CH(Me), C(Me)2, CH:NOR2, SO2, SO, S, CO, O, N(R2), CONH, NHCO; M = a heteroaryl moiety; n = 0-4; p = 0-5; X = Br, Cl, F, CF3, OH, OCF2H, OCF3, alkoxy, alkyl, cycloalkyl, cycloalkyloxy, heteroalkyl, CON(R7)2, SO2R2, OSO2R2, wherein X is independently selected when p>1; Y = a covalent bond, CH2, SO2, CO; Z = a covalent bond, CH2, SO2, or CO; some provisos are applied] are prepared Disclosed is a method of stimulating cannabinoid CB2 receptors in a patient comprising administering to a patient having CB2 receptors a CB2 receptor stimulating amount of one or more compds. I. Also disclosed is a method of treating cancer, inflammatory diseases, immunomodulatory diseases, or respiratory diseases comprising administering to a patient in need of such treatment one or more compds. I. The said cancer, inflammatory diseases, immunomodulatory diseases or respiratory diseases are one or more diseases selected from the group consisting of cutaneous T cell lymphoma, rheumatoid arthritis, systemic lupus erythematosus, multiple sclerosis, glaucoma, diabetes, osteoporosis, renal ischemia, myocardial infarction, cerebral stroke, cerebral ischemia, nephritis, hepatitis, glomerulonephritis, cryptogenic fibrosing aveolitis, psoriasis, atopic dermatitis, vasculitis, allergy, seasonal allergic rhinitis, Crohn's disease, inflammatory bowel disease, reversible airway obstruction, adult respiratory distress syndrome, asthma, chronic obstructive pulmonary disease (COPD), and bronchitis.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 10 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:991176 HCAPLUS Full-text

DOCUMENT NUMBER: 140:27654  
 TITLE: Preparation of N-( $\alpha$ -methylbenzyl) sulfonamides  
 as cannabinoid receptor ligands  
 INVENTOR(S): Kozlowski, Joseph A.; Shih, Neng-Yang; Lavey, Brian  
 J.; Rizvi, Razia K.; Shankar, Bandarpalle B.; Spitler,  
 James M.; **Tong, Ling**; Wolin, Ronald L.;  
 Wong, Michael K.  
 PATENT ASSIGNEE(S): Schering Corporation, USA  
 SOURCE: U.S. Pat. Appl. Publ., 68 pp., Cont.-in-part of U.S.  
 Ser. No. 72,354.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003232859	A1	20031218	US 2002-214897	20020807
US 2003096844	A1	20030522	US 2002-72354	20020206
ZA 2003005933	A	20041101	ZA 2003-5933	20030731
CA 2494827	AA	20040219	CA 2003-2494827	20030805
WO 2004014825	A1	20040219	WO 2003-US24398	20030805
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1539662	A1	20050615	EP 2003-784905	20030805
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005534715	T2	20051117	JP 2004-527741	20030805
US 2006009528	A1	20060112	US 2005-203946	20050815
PRIORITY APPLN. INFO.:				
				P 20010208
				A2 20020206
				P 20010522
				A 20020807
				W 20030805
OTHER SOURCE(S): MARPAT 140:27654				
GI				



AB Title compds. [I; R1 = H, alkyl, haloalkyl, cycloalkyl, cycloalkylamino, aralkyl, heteroaryl, amino, (substituted) aryl, etc.; R2, R5, R6 = H, alkyl; R3 = H, alkyl, Cl, F, CF3, OCF2H, OCF3, OH, alkoxy; R4 = H, (substituted) alkyl, alkoxy, cycloalkyl, alkenyl, aryl, PhCH2, heteroaryl, arylamino, heteroaryl amino, cycloalkyl amino, etc.; L1 = alkylene, alkenylene, CO, C(R2)2, CHOR2, NOR5, SO2, SO, S, O, NR2, NR2CO, CHCF3, CF2; L2 = bond, alkylene, CO, C(R2)2, NR2, NR2SO2, CONR2, S, SO, SO2, NOR5, CR2OH, etc.; X = H, halo, CF3, cyano, OCF2H, OCF3, alkyl, cycloalkyl, cycloalkoxy, alkoxy, heteroalkyl, CO2R2, NHR2, arylamino, OSO2R2, etc.; Y, Z = bond, CH2, SO2, CO; R1YNZR2 = atoms to form a heterocycle; n = 0-4], were prepared for treatment of cancer, inflammatory disease, immunomodulatory disease, or respiratory disease (no data). Thus, (S)- $\alpha$ -methylbenzylamine was stirred with (F3CCO)2O in CH2Cl2; the mixture was then treated with MeSO3H and dibromodimethylhydantoin to give 32% intermediate (II). II in THF at -78° was treated with MeLi and then with 4-MeOC6H4SO2Cl followed by warming to room temperature to give 65% di-Ph sulfone derivative. The latter in THF at -78° was treated with BuLi then with bis(4-methoxyphenyl)disulfide to give crude disulfide coupling product, which was treated with MCPBA in CH2Cl2 to give 45% bissulfone. This was deprotected with LiOH in H2O/dioxane followed by treatment with MeSO2Cl to give title compound (III). Pharmaceutical compns. comprising the compound I are claimed.

L23 ANSWER 11 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:629186 HCAPLUS Full-text

DOCUMENT NUMBER: 140:213341

TITLE: Extracting sapogenins from *Dioscorea zingiberensis* through enzymatic hydrolysis

AUTHOR(S): **Tong, Ling**; Zhang, Sheng-Ke; Li, Jin; Li, Bao-Lin

CORPORATE SOURCE: College of Chemistry and Materials Science, Shaanxi Normal University, Xi'an, 710062, Peop. Rep. China

SOURCE: Shaanxi Shifan Daxue Xuebao, Ziran Kexueban (2003), 31(2), 81-83

CODEN: SSDKF2

PUBLISHER: Shaanxi Shifan Daxue

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The method of extracting sapogenins from *dioscorea zingiberensis* through enzymic hydrolysis by orthogonal tests is presented. Under the condition of 3.0 mL of amylase, 350 mL of water and the reaction time of 12 h, the yield rate sapogenins in average is 2.37%, which is higher than the method of directive hydrolysis (the rate of yield for sapogenins is 1.84%).



L23 ANSWER 12 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:396851 HCAPLUS Full-text

DOCUMENT NUMBER: 138:401607

TITLE: Preparation of piperidino cannabinoid receptor ligands

INVENTOR(S): Friary, Richard J.; Kozlowski, Joseph A.; Shankar, Bandarpalle B.; Wong, Michael K. C.; Zhou, Guowel; Lavey, Brian J.; Shih, Neng-Yang; **Tong, Ling**; Chen, Lei; Shu, Youheng

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 148 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

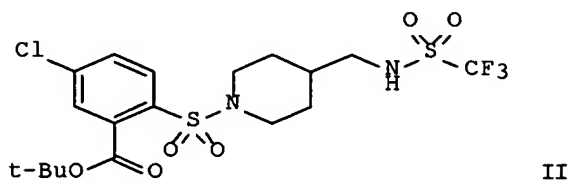
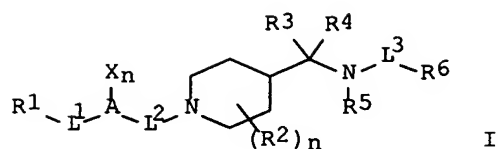
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003042174	A1	20030522	WO 2002-US36185	20021112
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2466440	AA	20030522	CA 2002-2466440	20021112
US 2004010013	A1	20040115	US 2002-292778	20021112
EP 1444203	A1	20040811	EP 2002-784433	20021112
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002014164	A	20040928	BR 2002-14164	20021112
JP 2005509032	T2	20050407	JP 2003-544011	20021112
NZ 532291	A	20051125	NZ 2002-532291	20021112
ZA 2004003685	A	20050523	ZA 2004-3685	20040513
NO 2004002435	A	20040611	NO 2004-2435	20040611
US 2005282861	A1	20051222	US 2005-197979	20050805
PRIORITY APPLN. INFO.:			US 2001-332911P	P 20011114
			US 2002-292778	A3 20021112
			WO 2002-US36185	W 20021112

OTHER SOURCE(S): MARPAT 138:401607

GI



AB Title compds. I [L1 = bond, CH<sub>2</sub>, CO, CO<sub>2</sub>, SO<sub>2</sub>, etc.; L2 = CH<sub>2</sub>, CH(alkyl), C(alkyl)<sub>2</sub>, etc.; L3 = bond, CO, SO<sub>2</sub>; R1 = H, halo, alkyl, haloalkyl, cycloalkyl, etc.; R2 = H, OH, halo, CF<sub>3</sub>, alkoxy, etc.; R3-4 = H, alkyl, taken together form a carbonyl group; R5 = H, alkyl; R6 = H, alkyl, haloalkyl, cycloalkyl, amino, etc.; n = 0-3] are prepared For instance, 4-(trifluoroacetamidomethyl)piperidine•TFA salt is reacted with p-chlorobenzenesulfonyl chloride (CH<sub>2</sub>Cl<sub>2</sub>, Et<sub>3</sub>N), the resulting sulfonamide functionalized ortho to the sulfonyl group (THF, n-BuLi, Boc<sub>2</sub>O), the trifluoroacetyl group removed (MeOH, K<sub>2</sub>CO<sub>3</sub>) and the amine refunctionalized with trifluoromethanesulfonic anhydride to give II. Compds. of the invention are found to exhibit cannabinoid CB<sub>2</sub> receptor binding activity in the range of 0.1 to 1000 nM and possess anti-inflammatory and immunomodulatory activity.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 13 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:29064 HCAPLUS Full-text  
 DOCUMENT NUMBER: 138:82568  
 TITLE: Determination of metals in nickel hydroxide by ICP-AES  
 AUTHOR(S): Tong, Jian; **Tong, Ling**  
 CORPORATE SOURCE: Beijing General Research Institute for Non-ferrous Metals, Beijing, 100088, Peop. Rep. China  
 SOURCE: Fenxi Shiyanshi (2002), 21(6), 44-46  
 CODEN: FENSE4; ISSN: 1000-0720  
 PUBLISHER: Fenxi Shiyanshi Bianjibu  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese

AB The determination of Zn, Co, Ca, Mg, Mn, Cd in nickel hydroxide was performed by inductive coupled plasma optical emission spectrometry (ICP-AES). Recovery of the method was between 95.9% .apprx. 103%, and RSD 0.93% .apprx. 18%.

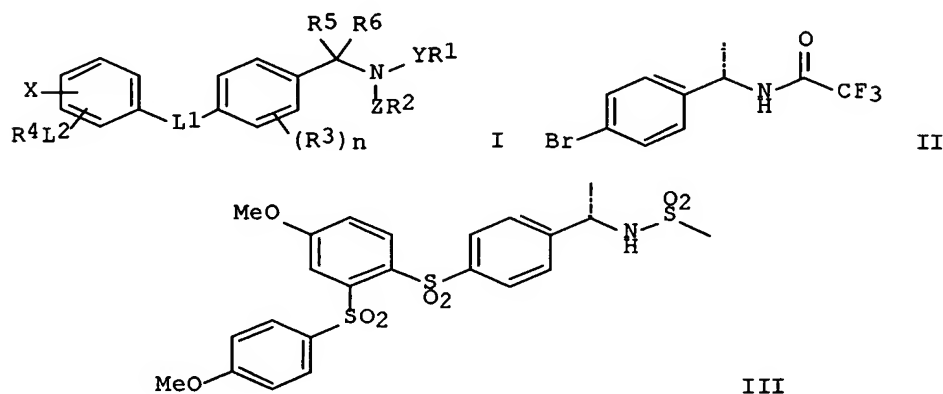
L23 ANSWER 14 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:615563 HCAPLUS Full-text  
 DOCUMENT NUMBER: 137:169310  
 TITLE: Preparation of α-methylbenzylsulfonamides as cannabinoid receptor ligands  
 INVENTOR(S): Kozlowski, Joseph A.; Shih, Neng-Yang; Lavey, Brian J.; Rizvi, Razia K.; Shankar, Bandarpalle B.; Spitler, James M.; **Tong, Ling**; Wolin, Ronald; Wong, Michael K.  
 PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 134 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002062750	A1	20020815	WO 2002-US3672	20020207
WO 2002062750	C2	20030918		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2436659	AA	20020815	CA 2002-2436659	20020207
EP 1368308	A1	20031210	EP 2002-740074	20020207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002006955	A	20040309	BR 2002-6955	20020207
JP 2004530649	T2	20041007	JP 2002-562710	20020207
NZ 526782	A	20050527	NZ 2002-526782	20020207
ZA 2003005933	A	20041101	ZA 2003-5933	20030731
NO 2003003505	A	20031007	NO 2003-3505	20030807
US 2006009528	A1	20060112	US 2005-203946	20050815
PRIORITY APPLN. INFO.:			US 2001-267375P	P 20010208
			US 2001-292600P	P 20010522
			US 2002-72354	A3 20020206
			WO 2002-US3672	W 20020207

OTHER SOURCE(S): MARPAT 137:169310  
 GI



AB Title compds. [I; R1 = H, alkyl, haloalkyl, cycloalkyl, cycloalkylamino, aralkyl, heteroaryl, amino, (substituted) aryl, etc.; R2, R5, R6 = H, alkyl; R3 = H, alkyl, Cl, F, CF3, OCF2H, OCF3, OH, alkoxy; R4 = H, (substituted) alkyl, alkoxy, cycloalkyl, alkenyl, aryl, PhCH2, heteroaryl, arylamino,

heteroarylamino, cycloalkylamino, etc.; L1 = alkylene, alkenylene, CO, C(R2)2, CHOR2, NOR5, SO2, SO, S, O, NR2, NR2CO, CHCF3, CF2; L2 = bond, alkylene, CO, C(R2)2, NR2, NR2SO2, CONR2, S, SO, SO2, NOR5, CR2OH, etc.; X = H, halo, CF3, cyano, OCF2H, OCF3, alkyl, cycloalkyl, cycloalkoxy, alkoxy, heteroalkyl, CO2R2, NHR2, arylamino, OSO2R2, etc.; Y, Z = bond, CH2, SO2, CO; R1YNZR2 = atoms to form a heterocycle; n = 0-4], were prepared for treatment of cancer, inflammatory disease, immunomodulatory disease, or respiratory disease (no data). Thus, (S)- $\alpha$ -methylbenzylamine was stirred with (F3CCO)2O in CH2Cl2; the mixture was then treated with MeSO3H and dibromodimethylhydantoin to give 32% intermediate (II). II in THF at -78° was treated with MeLi and then with 4-MeOC6H4SO2Cl followed by warming to room temperature to give 65% di-Ph sulfone derivative. The latter in THF at -78° was treated with BuLi then with bis(4-methoxyphenyl)disulfide to give crude disulfide coupling product, which was treated with MCPBA in CH2Cl2 to give 45% bissulfone. This was deprotected with LiOH in H2O/dioxane followed by treatment with MeSO2Cl to give title compound (III).

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 15 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:216511 HCAPLUS Full-text

DOCUMENT NUMBER: 132:231177

TITLE: Determination of trace arsenic in palladium chloride catalyst by GFAAS

AUTHOR(S): Wu, Xin-you; Zheng, Yong-zhang; Cai, Shao-qin; **Tong, Ling**; Li, Man-zhi

CORPORATE SOURCE: Gen. Res. Inst. Non-ferrous Metals, Beijing, 100088, Peop. Rep. China

SOURCE: Fenxi Shiyanshi (2000), 19(1), 33-35  
CODEN: FENSE4; ISSN: 1000-0720

PUBLISHER: Beijing Daxue Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The anal. method for trace As in PdCl2 catalyst by GFAAS was studied. The optimum parameters for graphite furnace with AAS were selected. Vitamin C was used as a matrix modifier. The proposed method is fast, convenient and has less interferences. The limit of detection is 5 $\mu$ g/L and the linear range is 2.5-50ng/g. The method was used to determine trace As in PdCl2 with satisfactory results.

L23 ANSWER 16 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:690856 HCAPLUS Full-text

DOCUMENT NUMBER: 130:24811

TITLE: Syntheses and structural studies of large, cleft-containing polyphenyl aromatic compounds

AUTHOR(S): **Tong, Ling**

CORPORATE SOURCE: Princeton Univ., Princeton, NJ, USA

SOURCE: (1998) 197 pp. Avail.: UMI, Order No. DA9833118  
From: Diss. Abstr. Int., B 1998, 59(5), 2211

DOCUMENT TYPE: Dissertation

LANGUAGE: English

AB Unavailable

L23 ANSWER 17 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:376476 HCAPLUS Full-text

DOCUMENT NUMBER: 129:95133

TITLE: Polyphenylbiphenyls and Polyphenylfluorenes

AUTHOR(S): **Tong, Ling**; Lau, Heidi; Ho, Douglas M.;

Pascal, Robert A., Jr.  
 CORPORATE SOURCE: Department of Chemistry, Princeton University,  
 Princeton, NJ, 08544, USA  
 SOURCE: Journal of the American Chemical Society (1998),  
 120(24), 6000-6006  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A series of highly congested polyphenylbiphenyls and polyarylfluorenes has been prepared and their X-ray structures determined. Decaphenylbiphenyl adopts a very unusual C<sub>1</sub>-sym. geometry (rather than the more intuitive D<sub>2</sub> geometry) in which one of the central benzene rings is distorted into a boat conformation. AM1 calcns. confirm that the C<sub>1</sub> geometry is the ground state but indicate that less highly substituted biphenyls should adopt D<sub>2</sub> geometries. The structure of 2,2',4,4',6,6'-hexaphenylbiphenyl supports the latter prediction; this material has crystallog. C<sub>2</sub> symmetry and (except for the orientation of the para Ph groups) approx. D<sub>2</sub> symmetry in the solid state. Octaphenylfluorenone has been prepared in four steps from tetraphenylcyclopentadienone. Its X-ray structure shows the fluorenone core to be twisted and sterically shielded by the eight peripheral Ph groups; nevertheless, phenylmagnesium bromide adds easily to the carbonyl group of its equally hindered di-Me derivative, 2,3,5,6,7,8-hexaphenyl-1,4-di(p-tolyl)fluorenone. Reduction of the resulting fluorenone with TiCl<sub>3</sub> gives a nonaarylfluorene, 2,3,5,6,7,8,9-heptaphenyl-1,4-di(p-tolyl)fluorene, and its X-ray structure shows distortions similar to those of octaphenylfluorenone.  
 REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 18 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:523697 HCAPLUS Full-text  
 DOCUMENT NUMBER: 127:218795  
 TITLE: Change of plasma endothelin (ET), calcitonin gene related peptide (CGRP) and substance P levels between patients with painless or with painful myocardial ischemia  
 AUTHOR(S): Li, Dayuan; Zhang, Junhua; Tong, Ling; Shao, Geng; Ding, Wenhui; Li, Jing  
 CORPORATE SOURCE: Department of Cardiology, First Affiliated Hospital, Beijing Medical University, Beijing, 100034, Peop. Rep. China  
 SOURCE: Zhongguo Bingli Shengli Zazhi (1996), 12(4), 396-398  
 CODEN: ZBSZEB; ISSN: 1000-4718  
 PUBLISHER: Jinan Daxue  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese

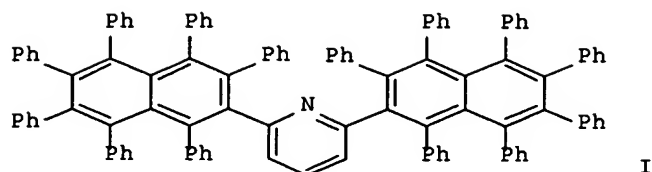
AB In 15 painless patients (group 1), 11 patients with pain (group 2) and 7 healthy controls (group 3), the plasma levels of ET, CGRP and substance P were measured by RIA at resting state and immediately after exercise test. No statistical differences in all resting plasma ET, CGRP and substance P levels among the three groups were found. The plasma CGRP levels among the 3 groups were not significantly different after exercise. After exercise, the plasma levels of ET in groups 1, 2 and 3 were 77.70 ± 18.44, 111.33 ± 24.82 and 94.38 ± 12.59 ng L<sup>-1</sup>, resp., while the plasma levels of substance P in groups 1, 2 and 3 were 2.25 ± 0.21, 2.46 ± 0.20 and 2.18 ± 0.16 nmol L<sup>-1</sup>, resp. Both the plasma levels of ET and substance P in group 2 was significantly higher than those in groups 1 and 3 (P > 0.01 and P < 0.05, resp.). The results suggest that painful myocardial ischemia may be related to the increase of plasma levels of ET and substance P, while in painless myocardial ischemia plasma levels of ET and substance P were not changed.

L23 ANSWER 19 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1997:510215 HCAPLUS Full-text  
 DOCUMENT NUMBER: 127:135588  
 TITLE: The Albatrossenes: Large, Cleft-Containing, Polyphenyl  
 Polycyclic Aromatic Hydrocarbons  
 AUTHOR(S): **Tong, Ling**; Ho, Douglas M.; Vogelaar, Nancy  
 J.; Schutt, Clarence E.; Pascal, Robert A., Jr.  
 CORPORATE SOURCE: Department of Chemistry, Princeton University,  
 Princeton, NJ, 08544, USA  
 SOURCE: Journal of the American Chemical Society (1997),  
 119(31), 7291-7302  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The syntheses and x-ray structures of very large polycyclic aromatic compds. containing clefts defined by polyphenylaryl groups are described. The C2-sym. albatrossenes 1,3-bis(heptaphenyl-2-naphthyl)benzene (I) and 1,3-bis(heptaphenyl-1-naphthyl)benzene (II), as well as brominated derivs., were synthesized by the addition of tetraphenylbenzyne to the appropriate polyphenyl biscyclopentadienones. The 2-naphthyl isomers have wide, shallow clefts, and the 1-naphthyl isomers have deep, narrow clefts, which were observed to change size dramatically in different crystal environments. In a similar way, 1,3,5-tris(pentaphenylphenyl)benzene (III), a D3-sym. mol. propeller with a diameter of 21 Å, and 1,3,5-tris(heptaphenyl-2-naphthyl)benzene (IV) were prepared by the addition of diphenylacetylene and tetraphenylbenzyne, resp., to a triscyclopentadienone.

L23 ANSWER 20 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1997:18701 HCAPLUS Full-text  
 DOCUMENT NUMBER: 126:199431  
 TITLE: Albatrossidine: a large, easily synthesized molecular  
 cleft  
 AUTHOR(S): **Tong, Ling**; Ho, Douglas M.; Vogelaar, Nancy  
 J.; Schutt, Clarence E.; Pascal, Robert A., Jr.  
 CORPORATE SOURCE: Dep. Chemistry, Princeton Univ., Princeton, NJ, 08544,  
 USA  
 SOURCE: Tetrahedron Letters (1997), 38(1), 7-10  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The title compound, 2,6-bis(heptaphenyl-2-naphthalenyl)pyridine was (albatrossidine) (I) prepared in three steps from 2,6-bis(phenylethynyl)pyridine, and its x-ray structure was determined. The pyridine nitrogen lies at the base of a broad, chiral mol. cleft created by the perphenylnaphthyl wings of I.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 21 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:482109 HCAPLUS Full-text

DOCUMENT NUMBER: 125:162307

TITLE: Prognostic value of normal exercise myocardial perfusion imaging

AUTHOR(S): Lin, Jinghui; Zhu, Mei; Wu, Shuyan; Pan, Zhongyun; Li, Lin; Ruxian, Guli; Wang, Yanfu; Nie, Tao; Yang, Hu; Tong, Ling

CORPORATE SOURCE: The First Hospital, Beijing Medical University, Beijing, 100034, Peop. Rep. China

SOURCE: Zhonghua Heyixue Zazhi (1996), 16(1), 8-10

CODEN: CITCDE; ISSN: 0253-9780

PUBLISHER: Jiangsusheng Yuanzi Yixue Yanjiuso

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB 54 Patients underwent exercise myocardial perfusion imaging and exercise ECG test. The images of all of them were normal. Coronary arteriogram was performed in 50 patients. The likelihood of coronary artery disease (CAD LK) was estimated before and after the test by Bayesian anal. The difference between the CAD LK pre- and post-test was significant. The results suggest that a normal stress myocardial imaging can predict an excellent prognosis even in patients with CAD or a high pretest CAD LK or a pos. exercise ECG.

L23 ANSWER 22 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:176939 HCAPLUS Full-text

DOCUMENT NUMBER: 120:176939

TITLE: Fluorescence lifetimes of substituted indoles in solution and in free jets: evidence for intramolecular charge-transfer quenching

AUTHOR(S): Arnold, Steven; Tong, Ling; Sulkes, Mark

CORPORATE SOURCE: Department of Chemistry, Tulane University, New Orleans, LA, 70118, USA

SOURCE: Journal of Physical Chemistry (1994), 98(9), 2325-7

CODEN: JPCHAX; ISSN: 0022-3654

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fluorescence lifetime measurements for a variety of substituted indoles were taken in cyclohexane and in supersonic gas expansions. When the two data sets were compared, a strong trend became evident. Solvent polarizability effects can be seen as stabilizing intramol. charge-transfer quenching processes in

the substituted indoles that are stimulated by the correct placement of charge accepting/releasing substituents.

L23 ANSWER 23 OF 23 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:173083 HCAPLUS Full-text

DOCUMENT NUMBER: 116:173083

TITLE: Errors of the endpoints in titrimetric analysis

AUTHOR(S): **Tong, Ling**; Tian, Yingchao; Yin, Jiayuan

CORPORATE SOURCE: Dep. Chem., Yunnan Univ., Kunming, Peop. Rep. China

SOURCE: Daxue Huaxue (1990), 5(5), 31-2

CODEN: DAHUEW; ISSN: 1000-8438

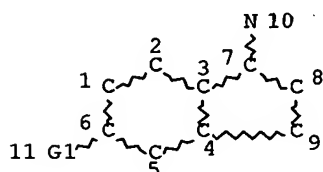
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The definition and calcn. equation derived from mol. ratio, reactant and elec. potential equilibrium for the endpoint errors in titrimetric anal. (e.g., acid-base, precipitation, oxidation-reduction, and complex-formation titrns.) are described and discussed with regard to teaching in anal. chemical

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L1 STR



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DEFAULT ECLEVEL IS LIMITED

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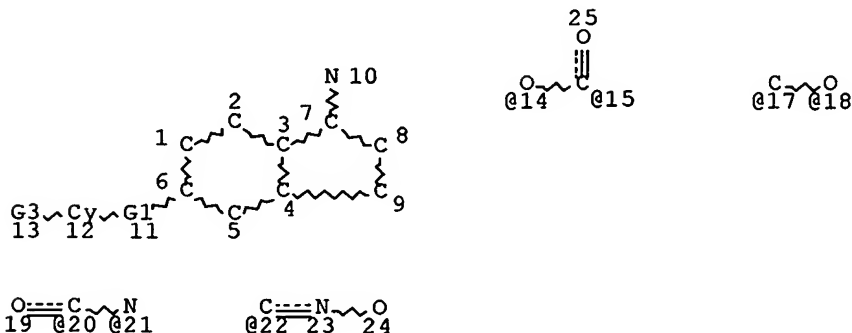
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NUMBER OF NODES IS 11

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L3 STR





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VAR G3=AK/CY/C/S/O/N

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

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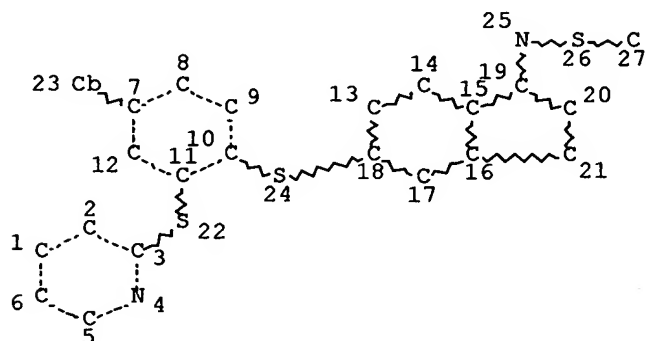
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NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L15 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L17 2 SEA FILE=REGISTRY SUB=L4 SSS FUL L15

L18 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L17

L19 205 SEA FILE=REGISTRY ABB=ON PLU=ON L4 NOT L17

L20 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L19

L21 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 NOT L18

L22 24 SEA FILE=HCAPLUS ABB=ON PLU=ON "TONG LING"/AU

L23 23 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 NOT (L18 OR L21)

L24 30 SEA FILE=HCAPLUS ABB=ON PLU=ON ("SHANKAR B"/AU OR "SHANKAR B B"/AU) OR ("SHANKAR BANDARPALLE"/AU OR "SHANKAR BANDARPALLE B"/AU OR "SHANKAR BANDERPALLE B"/AU) NOT (L18 OR L21 OR L23)

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L24 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:15012 HCAPLUS Full-text

TITLE: Cannabinoid receptor ligands

INVENTOR(S): Shankar, Bandarpalle B.; Gilbert, Eric;

Rizvi, Razia K.; Huang, Chunli; Kozlowski, Joseph A.;  
 McCombie, Stuart; Shih, Neng-Yang  
 PATENT ASSIGNEE(S): Schering Corporation, USA  
 SOURCE: PCT Int. Appl.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006002133	A1	20060105	WO 2005-US21870	20050621
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: US 2004-581837P P 20040622

AB Compounds of Formula (I) and/or pharmaceutically acceptable salts, solvates or prodrugs thereof, or pharmaceutical compositions containing such compounds exhibit anti-inflammatory and immunomodulatory activity, and can be effective as CB2 receptor ligands in treating cancer and inflammatory, immunomodulatory or respiratory diseases or conditions.

L24 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:588397 HCAPLUS Full-text

DOCUMENT NUMBER: 144:20516

TITLE: Role of tumor-derived transforming growth factor- $\beta$ 1 (TGF- $\beta$ 1) in site-dependent tumorigenicity of murine ascitic lymphosarcoma

AUTHOR(S): Thakur, V. S.; **Shankar, B.**; Chatterjee, S.;

Premachandran, S.; Sainis, K. B.

CORPORATE SOURCE: Radiation Biology & Health Sciences Division, Bioscience Group, Modular Laboratories, Bhabha Atomic Research Centre, Trombay, Mumbai, 400 085, India

SOURCE: Cancer Immunology Immunotherapy (2005), 54(9), 837-847  
 CODEN: CIIMDN; ISSN: 0340-7004

PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An ascitic lymphosarcoma (LS-A) of Swiss mice that regressed spontaneously on s.c. (s.c.) transplantation was investigated for the mechanism of its progressive growth and host mortality on i.p. (i.p.) transplantation. In vitro studies indicated significant inhibition of LS-A proliferation seeded at higher cell d. (>104/mL). Culture supernatants of LS-A caused bi-modal growth effects, the early supernatants (24 h) caused stimulation and the late (72 h) supernatants inhibited LS-A proliferation. The 72-h supernatants also suppressed T and B cell response to mitogens in a dose-dependent manner. Pan anti-transforming growth factor- $\beta$  antibody abrogated the inhibitory effects of supernatants. The supernatants contained both latent as well as bio-active

form of transforming growth factor- $\beta$ 1 (TGF- $\beta$ 1) as determined by ELISA. Mice bearing i.p. ascites tumor had elevated serum TGF- $\beta$ 1, hemoglobulinemia, splenic lymphopenia, impaired response of the T cells to mitogen and reduced expression of transferrin receptor (CD71) on the bone marrow cells. However, mice which rejected s.c. transplants, did not show significant changes in these parameters. Our studies indicated profound influence of site of tumor growth on tumor progression and host immune system mediated by tumor-derived TGF- $\beta$ 1. It is possible that human tumors which secrete TGF- $\beta$ 1 may exhibit similar patho-physiol. effects in the host depending on the anatomical site of the tumor.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:397173 HCAPLUS Full-text

DOCUMENT NUMBER: 143:371722

TITLE: Reductions in insecticide use from adoption of Bt cotton in South Africa: impacts on economic performance and toxic load to the environment  
AUTHOR(S): Bennett, R.; Ismael, Y.; Morse, S.; **Shankar, B.**

CORPORATE SOURCE: Department of Agricultural and Food Economics, The University of Reading, Reading, RG6 6AR, UK

SOURCE: Journal of Agricultural Science (2004), 142(6), 665-674.

CODEN: JASIAB; ISSN: 0021-8596

PUBLISHER: Cambridge University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The study reported presents the findings relating to com. growing of genetically-modified Bt cotton in South Africa by a large sample of smallholder farmers over three seasons (1998/99, 1999/2000, 2000/01) following adoption. The anal. presents constructs and compares groupwise differences for key variables in Bt v. non-Bt technol. and uses regressions to further analyze the production and profit impacts of Bt adoption. Anal. of the distribution of benefits between farmers due to the technol. is also presented. In parallel with these socio-economic measures, the toxic loads being presented to the environment following the introduction of Bt cotton are monitored in terms of insecticide active ingredient (ai) and the Biocide Index. The latter adjusts ai to allow for differing persistence and toxicity of insecticides. Results show substantial and significant financial benefits to smallholder cotton growers of adopting Bt cotton over three seasons in terms of increased yields, lower insecticide spray costs and higher gross margins. This includes one particularly wet, poor growing season. In addition, those with the smaller holdings appeared to benefit proportionately more from the technol. (in terms of higher gross margins) than those with larger holdings. Anal. using the Gini-coefficient suggests that the Bt technol. has helped to reduce inequality amongst smallholder cotton growers in Makhathini compared to what may have been the position if they had grown conventional cotton. However, while Bt growers applied lower amts. of insecticide and had lower Biocide Indexes (per ha) than growers of non-Bt cotton, some of this advantage was due to a reduction in non-bollworm insecticide. Indeed, the Biocide Index for all farmers in the population actually increased with the introduction of Bt cotton. The results indicate the complexity of such studies on the socio-economic and environmental impacts of GM varieties in the developing world.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

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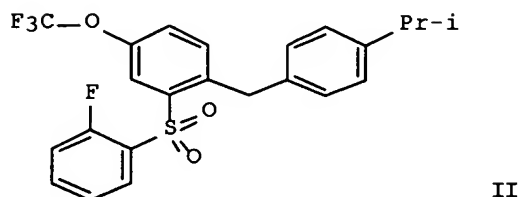
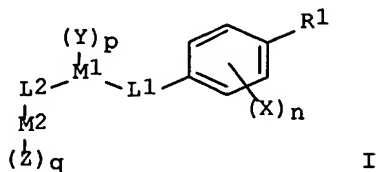
ACCESSION NUMBER: 2005:191340 HCAPLUS Full-text  
 TITLE: Identification of triaryl bis-sulfones as novel,  
 orally active cannabinoid-2 (CB2) receptor inverse  
 agonists  
 AUTHOR(S): Lavey, Brian J.; Zhou, Guowei; Spitler, James; Wu,  
 Jie; **Shankar, Bandarpalle**; Rizvi, Razia;  
 Yang, De-Yi; Kozlowski, Joseph; Hipkin, R. William;  
 Gonsiorek, Waldemar; Bober, Loretta; Fine, Jay;  
 Rojas-Triana, Alberto; Jackson, James V.; Fossetta,  
 James; Heimark, Larry; Clarke, Nigel; Wolin, Ronald;  
 Lundell, Daniel; Shih, Neng-Yang; Piwinski, John J.;  
 Narula, Satwant; Lunn, Charles A.  
 CORPORATE SOURCE: Department of Chemistry, Schering-Plough Research  
 Institute, Kenilworth, NJ, 07033-0539, USA  
 SOURCE: Abstracts of Papers, 229th ACS National Meeting, San  
 Diego, CA, United States, March 13-17, 2005 (2005),  
 MEDI-004. American Chemical Society: Washington, D.  
 C.  
 CODEN: 69GQMP  
 DOCUMENT TYPE: Conference; Meeting Abstract  
 LANGUAGE: English  
 AB Triaryl Bis-Sulfones have been identified as a new class of Cannabinoid-2  
 (CB2) inverse agonists. Compds. in the class are shown to have nanomolar  
 potency at CB2, high selectivity for CB2 in preference to CB1, and good plasma  
 levels after oral dosing.

L24 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:780365 HCAPLUS Full-text  
 DOCUMENT NUMBER: 141:295728  
 TITLE: Preparation of benzene derivatives as cannabinoid  
 receptor ligands  
 INVENTOR(S): **Shankar, Bandarpalle B.**; Rizvi, Razia K.;  
 Kozlowski, Joseph A.; Shih, Neng-Yang  
 PATENT ASSIGNEE(S): Schering Corporation, USA  
 SOURCE: U.S. Pat. Appl. Publ., 53 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004186148	A1	20040923	US 2004-803577	20040318
CA 2519401	AA	20041007	CA 2004-2519401	20040318
WO 2004085385	A2	20041007	WO 2004-US8333	20040318
WO 2004085385	A3	20041125		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1611090	A2	20060104	EP 2004-757826	20040318

10/721,015

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK  
 PRIORITY APPLN. INFO.: US 2003-456268P P 20030320  
 WO 2004-US8333 W 20040318  
 OTHER SOURCE(S): MARPAT 141:295728  
 GI



AB Compds. of the formula I [R1 = H, alkoxy, alkyl, aryl, etc.; X = H, alkoxy, cycloalkyl, aryl, etc.; Y = H, OH, CN, alkoxy, alkyl, etc.; Z = H, OH, CN, halo, alkoxy, etc.; L1 = bond, -CF2-, carbonyl, O, S, etc.; L2 = bond, carbonyl, S, SO, SO2, etc.; M1 = aryl cycloalkyl, heteroaryl, heterocycloalkyl; M2 = alkyl, aryl, cycloalkyl, heteroaryl, etc.; n = 0-4; p = 0-4; q = 0-5; with provisions] and the pharmaceutically acceptable salt or solvates thereof, are prepared and disclosed as possessing anti-inflammatory and immunomodulatory activity. Thus, e.g., II was prepared via addition of 4-isopropylphenyllithium (in situ generation from the aryl bromide) to 2-(2-fluorobenzyl)-4-trifluorobenzaldehyde, with subsequent reductive dehydroxylation and sulfur dioxidn. In cannabinoid receptor assays, I demonstrated Ki values ranging from 0.1 nM to 1000 nM. Also disclosed are pharmaceutical compns. containing said compds.

L24 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:34495 HCAPLUS Full-text

DOCUMENT NUMBER: 130:110148

TITLE: Process for preparing 1-(4-fluorophenyl)-3(R)-(3(S)-hydroxy-3-([phenyl or 4-fluorophenyl])-propyl)-4(S)-(4-hydroxyphenyl)-2-azetidinone

INVENTOR(S): Shankar, Bandarpalle B.

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: U.S., 6 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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10/721,015

US 5856473 A 19990105 US 1996-742012 19961031  
PRIORITY APPLN. INFO.: US 1996-742012 19961031  
OTHER SOURCE(S): CASREACT 130:110148; MARPAT 130:110148  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A process for preparing the title compound (I; X = H, F) comprises alkylation of a 3-unsubstituted chiral azetidinone (II) with cinnamyl bromide or 4-fluorocinnamyl bromide, Wacker oxidation of the product, reduction of the ketone product, and debenzylation of the resulting ketone. Thus, (S)-(+)-4-phenyl-2-oxazolidinone was N-alkylated with 5-(p-fluorophenyl)-4-pentenoic acid chloride in CH<sub>2</sub>Cl<sub>2</sub> containing DIPEA and DMAP to give the corresponding 1-acyloxazolidinone derivative, which was reacted with p-FC<sub>6</sub>H<sub>4</sub>N:CHC<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>Ph-p in CH<sub>2</sub>Cl<sub>2</sub>-H<sub>2</sub>O containing TiCl<sub>4</sub> and DIPEA to give the addition product III. This was treated with bis(trimethylsilyl)acetamide in toluene followed by TBAF to give the cyclized product IV, which was treated with Pd(OAc)<sub>2</sub>, benzoquinone, and perchloric acid in MeCN-H<sub>2</sub>O to give the ketone V. This was then treated with (R)-tetrahydro-1-methyl-3,3-dimethyl-1H,3H-pyrrolo[1,2-c][1,3,2]oxazaborole and borohydride-dimethyl sulfide complex in THF to give I (X = F).

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:257132 HCAPLUS Full-text

DOCUMENT NUMBER: 128:321585

TITLE: One pot solid phase synthesis of isoxazolines

AUTHOR(S): Shankar, B. B.; Yang, D. Y.; Girton, S.; Ganguly, A. K.

CORPORATE SOURCE: Schering-Plough Res. Inst., Kenilworth, NJ, 07033, USA

SOURCE: Tetrahedron Letters (1998), 39(17), 2447-2448

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1,3-Dipolar cycloaddn. of nitrile oxides generated in situ on solid phase in the presence of a variety of dipolaraphiles provided a library of isoxazolines and isoxazoles.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:809748 HCAPLUS Full-text

DOCUMENT NUMBER: 128:75317

TITLE: Substituted oximes, hydrazones and olefins as neurokinin antagonists

INVENTOR(S): Reichard, Gregory A.; Aslanian, Robert G.; Alaimo, Cheryl A.; Kirkup, Michael P.; Lupo, Andrew, Jr.; Mangiaracina, Pietro; McCormick, Kevin D.; Piwinski, John J.; Shankar, Bandarpalle B.; Shih, Neng-Yang; Spitler, James M.; Ting, Pauline C.; Ganguly, Ashit; Carruthers, Nicholas I.

PATENT ASSIGNEE(S): Schering Corp., USA

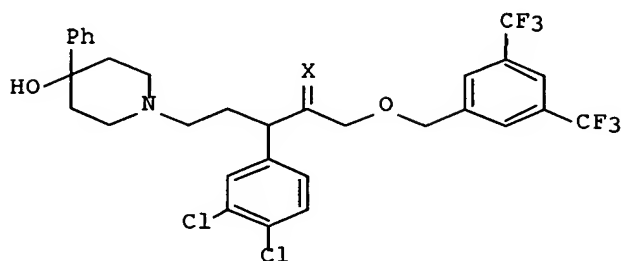
SOURCE: U.S., 80 pp., Cont.-in-part of U.S. Ser. No. 460,819, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5696267	A	19971209	US 1996-641384	19960430
CA 2218913	AA	19961107	CA 1996-2218913	19960501
CA 2218913	C	20030304		
CN 1189821	A	19980805	CN 1996-195172	19960501
CN 1134413	B	20040114		
ES 2158314	T3	20010901	ES 1996-915341	19960501
PT 823896	T	20011130	PT 1996-915341	19960501
US 5688960	A	19971118	US 1996-742013	19961031
US 5840725	A	19981124	US 1997-901028	19970725
PRIORITY APPLN. INFO.:			US 1995-432740	B2 19950502
			US 1995-460819	B2 19950601
			US 1996-641384	A2 19960430

OTHER SOURCE(S): MARPAT 128:75317  
 GI



I

AB Title compds. such as I (X = NOH, NNHCOMe, CHCH2NMe2) were prepared and tested as neurokinin-1, -2, and -3 receptor antagonists. NK1 activity was measured in guinea pigs, NK2 activity in the isolated hamster trachea. Thus, I (X = NOH) at 1 $\mu$ M showed 88.0 and 95.0% inhibition in NK1 and NK2 assays, resp.

L24 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1997:752780 HCAPLUS Full-text  
 DOCUMENT NUMBER: 128:22809  
 TITLE: Preparation of heteroarylketoximes and analogs as neurokinin antagonists  
 INVENTOR(S): Shankar, Bandarpalle B.  
 PATENT ASSIGNEE(S): Schering Corp., USA  
 SOURCE: U.S., 23 pp., Cont.-in-part of U.S. Ser. No. 641,384.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5688960	A	19971118	US 1996-742013	19961031

US 5696267	A	19971209	US 1996-641384	19960430
CN 1189821	A	19980805	CN 1996-195172	19960501
CN 1134413	B	20040114		
WO 9818785	A1	19980507	WO 1997-US18985	19971028
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9749916	A1	19980522	AU 1997-49916	19971028
AU 734309	B2	20010607		
EP 937064	A1	19990825	EP 1997-912826	19971028
EP 937064	B1	20021211		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, LT, LV, FI, RO				
JP 2000504341	T2	20000411	JP 1998-520559	19971028
JP 3152440	B2	20010403		
AT 229522	E	20021215	AT 1997-912826	19971028
ES 2184070	T3	20030401	ES 1997-912826	19971028
CA 2268847	C	20030527	CA 1997-2268847	19971028
CA 2268847	AA	19980507		
KR 2000052926	A	20000825	KR 1999-703796	19990429
PRIORITY APPLN. INFO.:				
			US 1995-432740	B2 19950502
			US 1995-460819	B2 19950601
			US 1996-641384	A2 19960430
			US 1996-742013	A 19961031
			WO 1997-US18985	W 19971028

OTHER SOURCE(S): MARPAT 128:22809

AB Z(CH<sub>2</sub>)<sub>a</sub>CRQC(:A)(CR<sub>6a</sub>R<sub>7a</sub>)dX(CR<sub>8a</sub>R<sub>9a</sub>)bT [I; A = NOR1, NNR2R3, etc.; Q = (un)substituted (hetero)aryl, etc.; R = H or (hydroxy)alkyl; R<sub>1</sub>-R<sub>3</sub> = H, (un)substituted alkyl, -(hetero)aryl, etc.; CR<sub>6a</sub>, R<sub>7a</sub>, CR<sub>8a</sub> = H, (hydroxy- or alkoxy)alkyl, (un)substituted Ph, etc.; R<sub>9a</sub> = groups cited for R<sub>6a</sub>, alkoxy, etc.; T = (un)substituted cycloalkyl, -(hetero)aryl, etc.; X = bond, O, CO, (alkyl)imino, etc.; Z = 4-hydroxy-4-phenylpiperidino, (un)substituted -4-(2-oxopyrrolidino)piperidino, etc.; a = 1-4; b, d = 0-2] were prepared. Thus, 3,5-(F3C)C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>Br was etherified by HOCH<sub>2</sub>CO<sub>2</sub>Me and the product condensed with 2-thiopheneacetic acid to give 3,5-(F3C)C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>OCH<sub>2</sub>C(:A)CHRQ (Q = 2-thienyl) (II; A = O, R = H) which was converted in 3 steps to II (A = NOME) (III; R = CH<sub>2</sub>CHO). The latter was reductively aminated by 4-hydroxy-4-phenylpiperidine to give III [R = 2-(4-hydroxy-4-phenylpiperidino)ethyl]. Data for biol. activity of I were given.

L24 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:643825 HCAPLUS Full-text

DOCUMENT NUMBER: 127:303048

TITLE: SCH 47112, a novel staurosporine derivative, inhibits 12-O-tetradecanoylphorbol-13-acetate-induced inflammation and epidermal hyperplasia in hairless mouse skin

AUTHOR(S): Reynolds, N. J.; McCombie, S. W.; Shankar, B. B.; Bishop, W. R.; Fisher, G. J.

CORPORATE SOURCE: Department of Dermatology, University of Michigan Medical School, Ann Arbor, MI, 48109-0609, USA

SOURCE: Archives of Dermatological Research (1997), 289(9), 540-546

CODEN: ADREDL; ISSN: 0340-3696

PUBLISHER: Springer



DOCUMENT TYPE: Journal

LANGUAGE: English

AB Protein kinase C (PKC) regulates keratinocyte growth and differentiation as well as inflammation in skin, processes which are abnormal in skin diseases such as psoriasis. 12-O-tetradecanoylphorbol-13-acetate (TPA) binds to and activates PKC. We investigated the effects of SCH 47112, a novel staurosporine derivative, which interactions with the catalytic domain on PKC, on TPA-induced inflammation and hyperplasia in hairless mouse skin and TPA-induced differentiation in cultured human keratinocytes. Dorsal mouse skin was treated with vehicle, TPA (2.0/2.5 nmol) or SCH 47112 followed by TPA. Epidermal thickness, and epidermal, upper dermal and deep dermal inflammation (assessed on an ordinal semiquant. scale) were determined in biopsies taken 24 h and 48 h post-treatment. SCH 47112 (100 nmol) inhibited TPA-induced epidermal, upper dermal and deep dermal inflammation by 71%, 45% and 22%, resp., at 24 h (n = 3, P < 0.05). TPA-induced epidermal hyperplasia was inhibited by SCH 47112 (400 nmol) by 38% at 48 h (n = 3, P < 0.05). In addition, in cultured human keratinocytes, SCH 47112 inhibited TPA induction of transglutaminase I protein, which catalyzes the formation of crosslinked envelopes. These results indicate that SCH 47112 exhibits biol. activity, inhibiting TPA-induced changes in hairless mouse skin in vivo and cultured human keratinocytes in vitro, and suggest that PKC inhibitors may have a therapeutic role in inflammatory skin diseases.

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:403182 HCAPLUS Full-text

DOCUMENT NUMBER: 127:17572

TITLE: Preparation of (R)-3-[(S)-3-hydroxy-3-phenylpropyl]-2-azetidinones

INVENTOR(S): Shankar, Bandarpalle B.

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 14 pp.

CODEN: PIXXD2

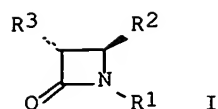
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9716424	A1	19970509	WO 1996-US17083	19961030
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9674728	A1	19970522	AU 1996-74728	19961030
PRIORITY APPLN. INFO.:			US 1995-6182P	P 19951102
			WO 1996-US17083	W 19961030
OTHER SOURCE(S):			CASREACT 127:17572; MARPAT 127:17572	
GI				



AB Title compds. (I; R1 = C6H4F-4; R2 = C6H4(OH)-4) [II; R3 = (S)-CH2CH2CH(OH)C6H4R-4; R = H or F] were prepared by, e.g., stereoselective alkenylation of II (R3 = H) by 4-RC6H4CH:CHCH2Br followed by oxidation to the ketone and stereoselective reduction

L24 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:26236 HCAPLUS Full-text

DOCUMENT NUMBER: 126:47113

TITLE: Substituted oximes, hydrazones and olefins as neurokinin antagonists

INVENTOR(S): Reichard, Gregory A.; Aslanian, Robert G.; Alaimo, Cheryl L.; Kirkup, Michael P.; Lupo, Andrew; Mangiaracina, Pietro; McCormick, Kevin D.; Piwinski, John J.; **Shankar, Bandarpalle**; et al.

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 21 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9634857	A1	19961107	WO 1996-US5659	19960501
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2218913	AA	19961107	CA 1996-2218913	19960501
CA 2218913	C	20030304		
AU 9657140	A1	19961121	AU 1996-57140	19960501
AU 706526	B2	19990617		
EP 823896	A1	19980218	EP 1996-915341	19960501
EP 823896	B1	20010711		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, LT, LV, FI				
JP 10506923	T2	19980707	JP 1996-533354	19960501
JP 3255421	B2	20020212		
CN 1189821	A	19980805	CN 1996-195172	19960501
CN 1134413	B	20040114		
BR 9608269	A	19990217	BR 1996-8269	19960501
NZ 307715	A	20000128	NZ 1996-307715	19960501
AT 203014	E	20010715	AT 1996-915341	19960501
ES 2158314	T3	20010901	ES 1996-915341	19960501
PT 823896	T	20011130	PT 1996-915341	19960501
NO 9705029	A	19971230	NO 1997-5029	19971031
NO 310189	B1	20010605		

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HK 1008221  
GR 3036676  
PRIORITY APPLN. INFO.:

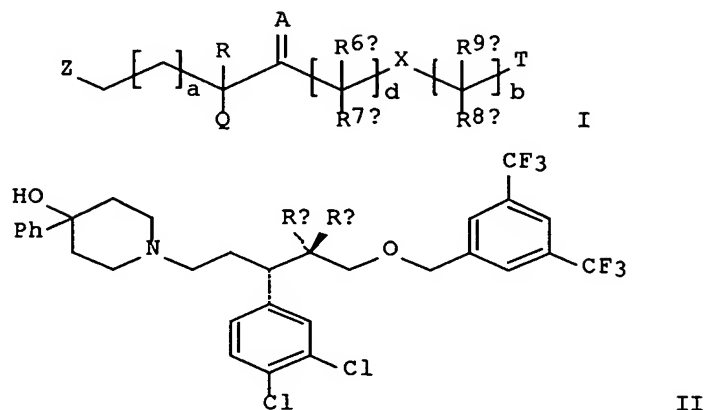
A1 20010928  
T3 20011231

HK 1998-109217  
GR 2001-401533  
US 1995-432740  
US 1995-460819  
WO 1996-US5659

19980717  
20010920  
A 19950502  
A 19950601  
W 19960501

OTHER SOURCE(S):  
GI

MARPAT 126:47113



AB Compds. I and their pharmaceutically acceptable salts are disclosed [wherein: a = 0-3; b, d, e = 0-2; R = H, C1-6 alkyl, OH, C2-6 hydroxyalkyl; A = (un)substituted oxime, hydrazone, or olefin; X = bond, CO, O, NR6, S(O)e, N(R6)CO, OCON(R6), OC(:S)NR6, N(R6)C(:S)O, C(:NOR1), S(O)2NR6, N(R6)S(O)2, N(R6)CO2, or OCO; T = H, phthalimidyl, aryl, heterocycloalkyl, heteroaryl, cycloalkyl, bridged cycloalkyl; Q = SR6, NJ(R6)(R7), OR6, Ph, naphthyl, or heteroaryl; R6a, R7a, R8a, R9a, R6 and R7 = H, C1-6 hydroxyalkyl, C1-6 alkoxy-C1-6 alkyl, Ph, CH2Ph; or NR6R7 forms a ring; R9a = R6 or OR6; Z = morpholinyl, (un)substituted piperazinyl, (un) substituted piperidino and analogs, substituted 8-azabicyclo[3.2.1]octan-8-yl; g = 0-3; h = 1-4; provided that (h + g) = 1-7]. Also disclosed are methods of treating asthma, cough, bronchospasm, inflammatory diseases, and gastrointestinal disorders with I, and pharmaceutical compns. comprising I. For instance, 3-(3,4-dichlorophenyl)-2-propenoic acid underwent a sequence of Me esterification (99%), reduction by Dibal-H to an alc. (99%), O-acetylation (97%), rearrangement (89%), epoxidn. and cyclization to form a furanone derivative (81%), and 3 addnl. steps (71%, 91%, and >90%), to give the epimeric alcs. II [Ra/Rb = H/OH or OH/H]. These underwent Jones oxidation to the ketone (82%), and oximation with MeONH2.HCl (67%), to give title compound II [RaRb = :NOMe] (III). Several bioassays were performed, and III at 1  $\mu$ M gave 88.0% inhibition at NK1 receptors and 95.0% inhibition at NK2 receptors.

L24 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:573166 HCAPLUS Full-text

DOCUMENT NUMBER: 125:292241

TITLE: (-)-SCH 57939: synthesis and pharmacological properties of a potent, metabolically stable cholesterol absorption inhibitor

AUTHOR(S): Kirkup, Michael P.; Rizvi, Razia; Shankar, Bandarpalle; Shankar, B.; Dugar, Sundeep; Clader, John W.; McCombie, Stuart W.; Lin, Sue-Ing; Yumibe, Nathan; et al.

CORPORATE SOURCE: Schering-Plough Res. Inst., Kenilworth, NJ, 07033, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1996),  
 6(17), 2069-2072  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Previous SAR studies of C-3 side chain modified analogs of (-)-SCH 48461, as well as information concerning the metabolic stability in this series, enabled us to design a cholesterol absorption inhibitor (i.e., (-)-SCH 57939) with tenfold higher potency and greatly enhanced metabolic stability. The synthesis and pharmacol. profile, including the role of relative stereochem. in determining the SAR of these compds., are discussed.

L24 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:376652 HCAPLUS Full-text

DOCUMENT NUMBER: 125:142356

TITLE: Synthesis of an optically pure 3-unsubstituted  $\beta$ -lactam via an asymmetric Reformatskii reaction and its conversion to cholesterol absorption inhibitors

AUTHOR(S): **Shankar, B. B.**; Kirkup, M. P.; McCombie, S. W.; Clader, J. W.; Ganguly, A. K.

CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Tetrahedron Letters (1996), 37(24), 4095-4098  
 CODEN: TELEAY; ISSN: 0040-4039

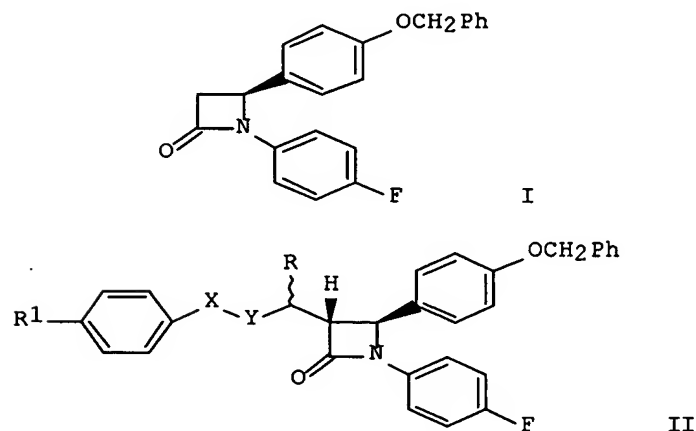
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:142356

GI



AB Asym. induction by several chiral alcs. in the reaction of their bromoacetates with imines in the presence of activated Zn (Reformatsky reaction) was studied. (-)-Trans-2-phenylcyclohexanol and (-)-phenylmenthol gave  $\beta$ -lactam I in >99% ee via cyclization of the diastereoisomeric  $\beta$ -aminoester

intermediates. The resulting chiral 3-unsubstituted azetidin-2-one I was converted to 3-substituted products II (R = OH, R1 = F, X = O, Y = CH2; R = R1 = H, XY = CH=CH, COCH2) which exhibit cholesterol absorption inhibitory activity (no data).

L24 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:242351 HCAPLUS Full-text  
 DOCUMENT NUMBER: 124:358960  
 TITLE: Synthesis, structure, and properties of  
 LaSr3Fe3-xGaxO10- $\delta$ : an intermediate Fe3+ spin  
 state  
 AUTHOR(S): **Shankar, B.**; Steinfink, H.  
 CORPORATE SOURCE: Dep. Chem. Eng. Mater. Sci. Eng. Program, Univ. Texas  
 Austin, Austin, TX, 78712, USA  
 SOURCE: Journal of Solid State Chemistry (1996), 122(2), 390-3  
 CODEN: JSSCBI; ISSN: 0022-4596  
 PUBLISHER: Academic  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB LaSr3Fe3-xGaxO10- $\delta$  (x = 0.2-2.0) were prepared from SrCO3, La2O3, Fe2O3 and Ga2O3 powders. The solid solubility of Ga in this solid solution extends to x = 2. A phase change occurs near the composition x = 1 from tetragonal to orthorhombic. A Rietveld x-ray powder diffraction structure determination of LaSr3FeGa2O9 indicates that Fe occupies the central octahedral interstice in the triple octahedral layer. O vacancies are present in the equatorial positions of the central octahedron and in the bridging O position. The phase change is driven by the increase of the c/a ratio of the tetragonal phase. The phases are antiferromagnets with Neel temps. of 45 K for the tetragonal phases that go to zero for the orthorhombic phase. The effective magnetic moment for the tetragonal phase is 6  $\mu$ B for high spin Fe3+. An intermediate spin state of 4  $\mu$ B is observed for the orthorhombic phase indicative of three unpaired electrons.

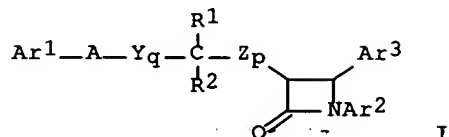
L24 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:995516 HCAPLUS Full-text  
 DOCUMENT NUMBER: 124:175683  
 TITLE: Substituted azetidinone compounds useful as  
 hypocholesterolemic agents  
 INVENTOR(S): Kirkup, Michael P.; Dugar, Sundeep; **Shankar,**  
**Banderpalle B.**  
 PATENT ASSIGNEE(S): Schering Corp., USA  
 SOURCE: PCT Int. Appl., 41 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9526334	A1	19951005	WO 1995-US3196	19950322
W:	AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN			
RW:	KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			

10/721,015

CA 2186364	AA	19951005	CA 1995-2186364	19950322
AU 9521596	A1	19951017	AU 1995-21596	19950322
AU 686361	B2	19980205		
EP 751934	A1	19970108	EP 1995-914719	19950322
EP 751934	B1	19990825		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
HU 74887	A2	19970228	HU 1996-2616	19950322
CN 1144522	A	19970305	CN 1995-192277	19950322
JP 09510970	T2	19971104	JP 1995-525184	19950322
JP 3524927	B2	20040510		
AT 183738	E	19990915	AT 1995-914719	19950322
ES 2135050	T3	19991016	ES 1995-914719	19950322
NO 9604008	A	19961122	NO 1996-4008	19960924
FI 9603817	A	19960925	FI 1996-3817	19960925
PRIORITY APPLN. INFO.:			US 1994-218498	A 19940325
			WO 1995-US3196	W 19950322
OTHER SOURCE(S):	CASREACT 124:175683; MARPAT 124:175683			
GI				



AB Substituted azetidinone hypocholesterolemic agents of formula (I) or a pharmaceutically acceptable salt thereof, wherein: Ar1 is R3-substituted aryl; Ar2 is R4-substituted aryl; Ar3 is R5-substituted aryl; Y and Z are independently-CH2-, -CH(lower alkyl)- or -C(dilower alkyl)-; A is -O-, -S-, -S(O)- or -S(O)2-; R1 is -OR6, -O(CO)R6, -O(CO)OR9 or -O(CO)NR6R7; R2 is hydrogen, lower alkyl or aryl; or R1 and R2 together are =O; q is 1, 2 or 3; p is 0, 1, 2, 3 or 4; R4 is 1-3 substituents independently selected from -OR6, -O(CO)R6, -O(CO)OR9, -O(CH2)1-5OR9, -O(CO)NR6R7, -NR6R7, -NR6(CO)R7, -NR6(CO)OR9, -NR6(CO)NR7R8, -NR6SO2-lower alkyl, -NR6SO2-aryl, -CONR6R7, -COR6, -SO2NR6R7, S(O)O-2-alkyl, S(O)O-2-aryl, -O(CH2)1-10-COOR6, -O(CH2)0-10CONR6R7, o-halogeno, m-halogeno, o-lower alkyl, m-lower alkyl, -(lower alkylene)-COOR6 and -CH=CH-COOR6; R3 and R4 are 1-3 substituents independently selected from R5, hydrogen, p-lower alkyl, aryl, -NO2, CF3 and p-halogeno; R6, R7 and R8 are hydrogen, lower alkyl, aryl or aryl-substituted lower alkyl; and R4 is lower alkyl, aryl or aryl-substituted lower alkyl; are disclosed, as well as method of lowering serum cholesterol by administering said compds., pharmaceutical compns. containing them, the combination of a substituted azetidinone and a cholesterol biosynthesis inhibitor for the treatment and prevention of atherosclerosis, novel intermediates and methods for preparing them.

L24 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:14288 HCAPLUS Full-text

DOCUMENT NUMBER: 122:81843

TITLE: Indolocarbazoles. 4. Synthetic studies towards staurosporine and tjipanazoles: reactions of indolocarbazole with glycals

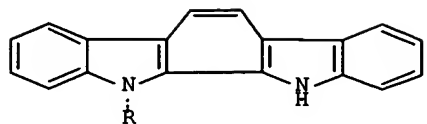
AUTHOR(S): Shankar, B. B.; McCombie, S. W.

CORPORATE SOURCE: Schering-Plough Res. Inst., Kenilworth, NJ, 07033, USA

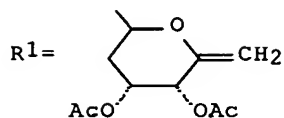
SOURCE: Tetrahedron Letters (1994), 35(19), 3005-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I



AB In an attempt to construct the unique N,N'-bidentate glycosyl linkage found in the staurosporine class of natural products, the first example of an acid catalyzed 2,6-condensation of an activated pyran and glycals with indolocarbazole I (R = H) is reported. Formation of novel unexpected products with 1,3-connections along with the expected product and its synthetic transformation to a potentially useful intermediate I (R = R1) are detailed.

L24 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:524570 HCAPLUS Full-text

DOCUMENT NUMBER: 121:124570

TITLE: Indolocarbazoles. 3. Synthesis of novel aza analogs of staurosporine and K 252a as PKC inhibitors

AUTHOR(S): Shankar, B. B.; Viet, A. Q.; Rizvi, R.;

Kirkup, M. P.; McCombie, S. W.; Ganguly, A. K.

CORPORATE SOURCE: Schering-Plough Res. Inst., Kenilworth, NJ, 07033, USA

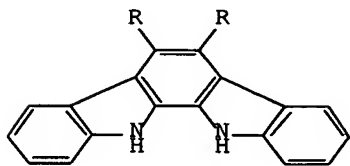
SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(3), 495-8

CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE: Journal

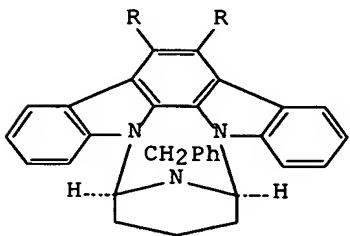
LANGUAGE: English

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I, R=H

II, RR=CONHCO



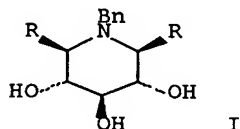
III, R=H

IV, RR=CONHCO

AB Indolocarbazole I and arcyrriaflavin A (II) reacted under basic conditions with 1-benzyl-2,6-bis(benzotriazolyl)piperidine to give III and IV. As an extension of this methodol. other related bis benzotriazole derivs. were synthesized and coupled with II to obtain a variety of aza derivs. N-benzoylation of these compds. gave novel PKC inhibitors.

L24 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:218333 HCAPLUS Full-text  
 DOCUMENT NUMBER: 120:218333  
 TITLE: A novel application of benzotriazole methodology: reactions of polyhydroxylated bis(benzotriazolyl)piperidines with mono- and bidentate nucleophiles  
 AUTHOR(S): **Shankar, B. B.**; Kirkup, M. P.; McCombie, S. W.; Ganguly, A. K.  
 CORPORATE SOURCE: Schering-Plough Res. Inst., Kenilworth, NJ, 07033, USA  
 SOURCE: Tetrahedron Letters (1993), 34(45), 7171-9  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 120:218333  
 GI



AB A variety of 2,6 substituted trihydroxy piperidines, e.g. I (R = H, Et, CN, MeS), were synthesized with stereocontrol from the corresponding 2,6 bis-(Benzotriazolyl) trihydroxy piperidine, which in turn was prepared from 1,2-O-isopropylidene-D-glucofuranose employing a simple, two step chemical manipulation. These products are potential glycosidase inhibitors and can be transformed to other useful chiral products.

L24 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:77509 HCAPLUS Full-text  
 DOCUMENT NUMBER: 120:77509  
 TITLE: Indolocarbazoles. 2. Synthetic studies towards staurosporine. An unexpected 1,2 migration of indolocarbazole nitrogen results in a novel and potent Protein Kinase C inhibitor  
 AUTHOR(S): **Shankar, B. B.**; McCombie, S. W.; Kirkup, M. P.; Viet, A. Q.; Puar, M. S.; Ganguly, A. K.  
 CORPORATE SOURCE: Schering-Plough Res. Inst., Kenilworth, NJ, 07033, USA  
 SOURCE: Tetrahedron Letters (1993), 34(36), 5685-8  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 120:77509  
 GI



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Attempted transformation of the readily accessible cyclofuransylated indolocarbazole I to a cyclopyranosylated compound related to II was explored. An unexpected rearranged product III was obtained from IV. Compound III was converted to V, a potent PKC inhibitor.

L24 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:517283 HCAPLUS Full-text

DOCUMENT NUMBER: 119:117283

TITLE: Preparation of 9,13-epoxy-1H,9H-diindolo[1,2,3-gh:3',2',1'-lm]pyrolo[3,4-j][1,7]benzodiazonine-1,3-diones and related compounds as antitumor and antipsoriatic agents

INVENTOR(S): McCombie, Stuart W.; Shankar, Bandarpalle B. ; Kirkup, Michael P.

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: Eur. Pat. Appl., 110 pp.

CODEN: EPXXDW

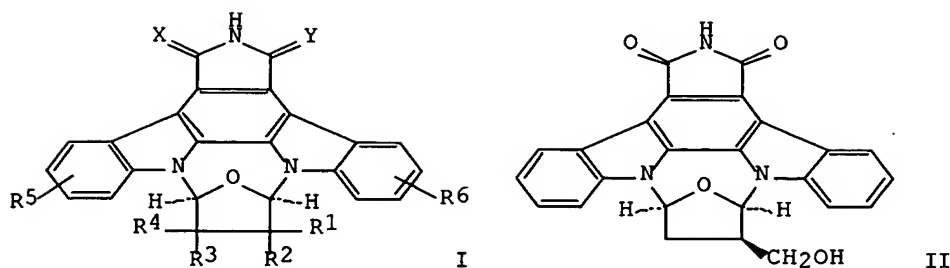
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 508792	A1	19921014	EP 1992-303187	19920409
R: PT				
CA 2108146	AA	19921012	CA 1992-2108146	19920409
WO 9218507	A1	19921029	WO 1992-US2661	19920409
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MW, NO, PL, RO, RU, SD, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE				
AU 9217982	A1	19921117	AU 1992-17982	19920409
AU 646163	B2	19940210		
EP 580812	A1	19940202	EP 1992-917468	19920409
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06503837	T2	19940428	JP 1992-510240	19920409
HU 70187	A2	19950928	HU 1993-2869	19920409
NO 9303611	A	19931008	NO 1993-3611	19931008
PRIORITY APPLN. INFO.:			US 1991-683770	A 19910411
			WO 1992-US2661	A 19920409
OTHER SOURCE(S):	MARPAT 119:117283			
GI				



AB Title compds. [I; X = O, S; Y = O, NH, (H, H), (H, OH), S; R1-R4 = H, CHO, cyano, carbamoyl, CO2H, alkoxy, carbonyl, CH:NNHCONH2, F, Cl, Br, OH, N3, SH, (substituted) alkyl, alkoxy, alkylthio, (acyl)amino, oximinomethyl, etc.; or R1R2, R3R4 = O, NOH, alkoxyimino, CH2, NNHCONH2; or R1R4 = bond; R5, R6 = H, F, Cl, Br, OH, N3, SH, (substituted) alkyl, alkoxy, alkylthio, (acyl)amino, etc.; with provisos], were prepared Thus, dibenzyl, indolo[2,3-a]carbazole-5,6-dicarboxylate was stirred 2 h with 2,5-dimethoxy-5-acetoxymethyltetrahydrofuran and 4-MeC6H4SO3H in CH2Cl2 to give the cycloaddn. product, which was heated with NH3 in Me2SO at 120° to give title compound II. I inhibited protein kinase C with IC50 = 0.5-230 nM.

L24 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:471341 HCAPLUS Full-text

DOCUMENT NUMBER: 115:71341

TITLE: Generation and in situ acylation of enaminone anions: a convenient synthesis of 3-carbethoxy-4(1H)-pyridinones and -4-pyrones and related compounds  
AUTHOR(S): McCombie, Stuart W.; Metz, William A.; Nazareno, Dennis; **Shankar, Bandarpalle B.**; Tagat, Jayaram

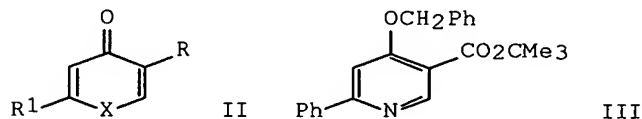
CORPORATE SOURCE: Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
SOURCE: Journal of Organic Chemistry (1991), 56(16), 4963-7  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

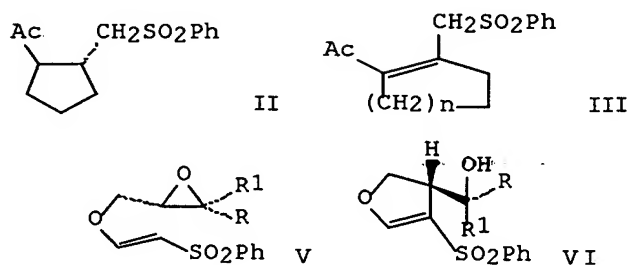
OTHER SOURCE(S): CASREACT 115:71341

GI



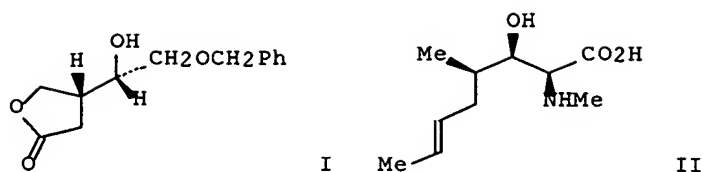
AB Acylation of oxobutanoates MeCOCR:CHNMe2 (I, R = CO2Et, CO2CMe3) with R1COCl (R1 = Ph, Me2CH, Me3C, PhCH:CH, MeCH:CH) in the presence of LiN(SiMe3)2 gives, after treatment with HCl/H2O or NH4OAc/HOAc, pyrone and pyridinone derivs. II (X = O, NH). Reacting I (R = SCH2Ph) with PhCOCl gave II (R = SCH2Ph, R1 = Ph, X = O). Alkylation of the pyridinone anions gives mixts. of N- and O-substituted compds. Thus, benzylation of II (R = CO2CMe3, R1 = Ph, X = NH) gave pyridine III and II (R = CO2Me3, R1 = Ph, X = NCH2Ph).

L24 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1991:408444 HCAPLUS Full-text  
 DOCUMENT NUMBER: 115:8444  
 TITLE: Alkylation of 2-oxy-substituted 1-sulfonylallyl and 1-sulfonylvinyl anions. New routes to functionalized carbocycles and dihydrofurans  
 AUTHOR(S): Padwa, Albert; Bullock, William H.; Dyszlewski, Andrew D.; McCombie, S. W.; Shankar, B. B.; Ganguly, A. K.  
 CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA  
 SOURCE: Journal of Organic Chemistry (1991), 56(11), 3556-64  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 115:8444  
 GI



AB Alkylation of PhSO<sub>2</sub>CHRC(OPh):CH<sub>2</sub> (I; R = H) with electrophiles proceeds  $\alpha$  to the phenylsulfonyl group to afford (I; R = alkyl, alkenyl, alkynyl). Reaction of I [R = (CH<sub>2</sub>)<sub>3</sub>CH:CH<sub>2</sub>, (CH<sub>2</sub>)<sub>n</sub>CH<sub>2</sub>CH<sub>2</sub>C.tplbond.CH; n = 1, 2] with PhSO<sub>2</sub>Na/HOAc gave cyclopentene II and cycloalkenes III, resp. Lithiation of (E)- or (Z)-ROCH:CR<sub>1</sub>SO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>R<sub>2</sub> (IV; R = Me, Et; R<sub>1</sub> = H; R<sub>2</sub> = H, Me) afforded the more stable (E)-IV (R<sub>1</sub> = Li) which reacted normally with aldehydes, ketones, alkyl halides, and epoxides. Thus, lithiation of oxiranylmethoxyvinyl sulfones V (R, R<sub>1</sub> = H, Me, Ph, CH<sub>2</sub>OCH<sub>2</sub>Ph) gave dihydrofurans VI.

L24 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1990:459795 HCAPLUS Full-text  
 DOCUMENT NUMBER: 113:59795  
 TITLE: Cyclofunctionalization of epoxy alcohol derivatives. 4. Cyclization of sulfonylacetate dianions: a synthesis of "MeBMT"  
 AUTHOR(S): McCombie, Stuart W.; Shankar, Bandarpalle B.; Ganguly, Ashit K.  
 CORPORATE SOURCE: Chem. Res., Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
 SOURCE: Tetrahedron Letters (1989), 30(50), 7029-32  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:59795  
 GI



AB     $\alpha,\alpha$ -Dianions, derived from arenesulfonylacetate esters of 2,3-epoxy alcs., cyclized to give 3-arenesulfonyl 4-(1-hydroxyalkyl)-  $\gamma$ -butyrolactones. Dianion fragmentation to regenerate the epoxy alc. was a competing, substrate-dependent process. Sulfonyllactone I was elaborated efficiently to an advanced intermediate for the unusual amino acid MeBMT (II) as well as to stereodefined cyclopropane derivs.

L24 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:459658 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 113:59658

TITLE: ~~A concise route to the oxathiazepine containing~~ ... ..  
eudistomin skeleton and some carba-analogs

AUTHOR(S): Kirkup, Michael P.; Shankar, B. B.;  
McCombie, Stuart; Ganguly, Ashit K.; McPhail, Andrew  
T.

CORPORATE SOURCE: Schering-Plough Corp., Bloomfield, NJ, 07003, USA

SOURCE: Tetrahedron Letters (1989), 30(49), 6809-12

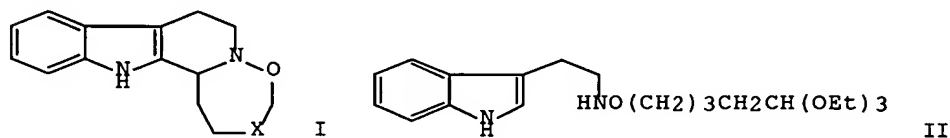
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:59658

GI



AB    The unsubstituted eudistomin skeleton containing the oxathiazepine D I (X = S) ring was prepared along with a series of unsubstituted and amino-substituted carba-analogs, e.g. I (X = CH<sub>2</sub>), using an intramol. Pictet-Spengler condensation of alkoxytryptamines, e.g. II. The structure of I (X = S) was determined by x-ray anal.

L24 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:496748 HCAPLUS [Full-text](#)

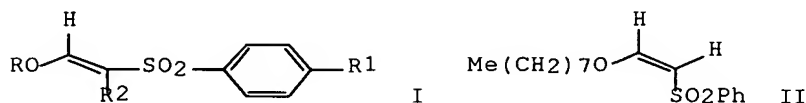
DOCUMENT NUMBER: 111:96748

TITLE: New sulfonylviny anion chemistry

AUTHOR(S): Shankar, Bandarpalle B.

CORPORATE SOURCE: Stevens Inst. Technol., Hoboken, NJ, USA  
 SOURCE: (1988) 109 pp. Avail.: Univ. Microfilms Int., Order No. DA8817326  
 From: Diss. Abstr. Int. B 1989, 49(7), 2656  
 DOCUMENT TYPE: Dissertation  
 LANGUAGE: English  
 AB Unavailable

L24 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1988:454407 HCAPLUS Full-text  
 DOCUMENT NUMBER: 109:54407  
 TITLE: Configurational properties and chemical reactivity of mono- and dianions derived from aryl 2-alkoxyvinyl sulfones  
 AUTHOR(S): McCombie, S. W.; **Shankar, B. B.**; Ganguly, A. K.; Padwa, Albert; Bullock, William H.; Dyszlewski, Andrew D.  
 CORPORATE SOURCE: Anti-Infect. Chem. Res., Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
 SOURCE: Tetrahedron Letters (1987), 28(36), 4127-30  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 109:54407  
 GI

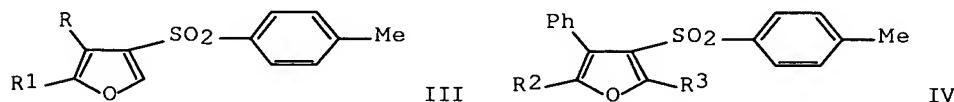


AB (E)-2-Alkoxy-1-arylsulfonyl ethenes I (R = Me, Et; R1 = Me, H; R2 = H) were regio- and stereospecifically lithiated at C-1 and the resulting species reacted with electrophiles to give synthetically useful products. E.g., the reaction of I (R = Et, R1 = Me) with BuLi followed by D2O gave 90% I (R = Et, R1 = Me, R2 = D). The reaction of (Z)-isomer II under similar conditions gave I (R = octyl, R1 = H, R2 = D).

L24 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1988:422698 HCAPLUS Full-text  
 DOCUMENT NUMBER: 109:22698  
 TITLE: Studies on lactams. Part 75. Stereocontrolled synthesis of  $\beta$ -lactams from amidomalonates: intermediates for thienamycin, carpetimycin and analogs  
 AUTHOR(S): Manhas, M. S.; Bhawal, B. M.; **Shankar, B. B.**; Bose, Ajay K.  
 CORPORATE SOURCE: Dep. Chem. Chem. Eng., Stevens Inst. Technol., Hoboken, NJ, 07030, USA  
 SOURCE: Journal of the Indian Chemical Society (1985), 62(11), 891-8  
 CODEN: JICSAH; ISSN: 0019-4522  
 DOCUMENT TYPE: Journal

LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 109:22698  
 GI For diagram(s), see printed CA Issue.  
 AB Complete stereocontrol of  $\beta$ -lactam formation is achieved by the intramol. cyclization of the epoxide of an N-acroylaminomalonate I ( $R = H, Me, R1 = Me, OMe$ ). The  $\beta$ -lactam so obtained is fused with a lactone ring II and selective hydrolysis of the lactone group leads to a trans  $\beta$ -lactam; selective decarboalkoxylation produces a cis  $\beta$ -lactam. The configuration of the carbinol side chain can be altered by a Mitsunobu reaction. The  $\pi$ -anisidino group is removed oxidatively to give N-unsubstituted  $\beta$ -lactams which are convenient intermediates for the carbapenem antibiotics, their epimers and analogs.

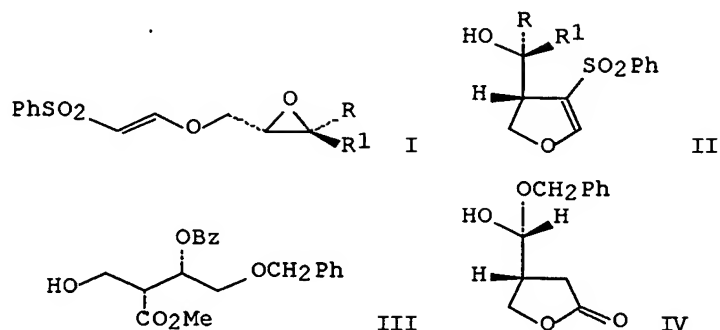
L24 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1988:150181 HCAPLUS Full-text  
 DOCUMENT NUMBER: 108:150181  
 TITLE: A new ring synthesis for 3- and polysubstituted furans: directing effects of a 3-(arenesulfonyl) group in metalation and Friedel-Crafts processes  
 AUTHOR(S): McCombie, S. W.; **Shankar, B. B.**; Ganguly, A. K.  
 CORPORATE SOURCE: Anti-Infect. Chem. Res., Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
 SOURCE: Tetrahedron Letters (1987), 28(36), 4123-6  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 108:150181  
 GI



AB The reaction of  $RCOCHR1Br$  [I;  $R = Ph, undecyl, Me; R1 = H, Me, Et; RR1 = (CH2)4$ ] with 4-MeC6H4SO2CH:CHO-K<sup>+</sup> gave  $RCOCHR1OCH:CHSO2C6H4Me-4$  (II). On treatment of II with  $LiN(CHMe2)2$  followed by 4-MeC6H4SO3H gave 62-72% yield tosylfurans III. Regiospecific alkylation of III ( $R = Ph, R1 = H$ ) gave 71% furan IV ( $R2 = H, R3 = Et$ ). Acylation of III ( $R = Ph, R1 = H$ ) with  $AcCl$  gave IV ( $R2 = Ac, R3 = H$ ).

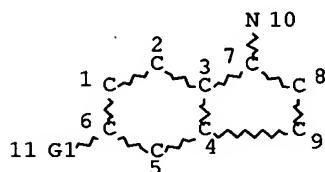
L24 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1987:4777 HCAPLUS Full-text  
 DOCUMENT NUMBER: 106:4777  
 TITLE: Cyclofunctionalization of epoxy alcohol derivatives.  
 1. Delivery of functionalized carbon for stereospecific synthesis of dihydrofurans and dihydroxy acids  
 AUTHOR(S): McCombie, Stuart W.; **Shankar, Bandarpalle B.**; Ganguly, Ashit K.  
 CORPORATE SOURCE: Schering-Plough Corp., Bloomfield, NJ, 07003, USA  
 SOURCE: Tetrahedron Letters (1985), 26(51), 6301-4  
 CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 106:4777  
 GI



AB E-2-(phenylsulfonyl)vinyl ethers of 2,3-epoxy alcs. I (R = H, Me, Ph, CH<sub>2</sub>OCH<sub>2</sub>Ph; R<sub>1</sub> = H, Me, Ph) were stereospecifically rearranged to dihydrofurans II on treatment with (Me<sub>2</sub>CH)<sub>2</sub>NLi. These compds. or derived des-sulfonyl compds. were converted to esters or lactones, e.g. III and IV, which correspond to regiospecific introduction of -CO<sub>2</sub>H or -CH<sub>2</sub>CO<sub>2</sub>H groups with inversion.

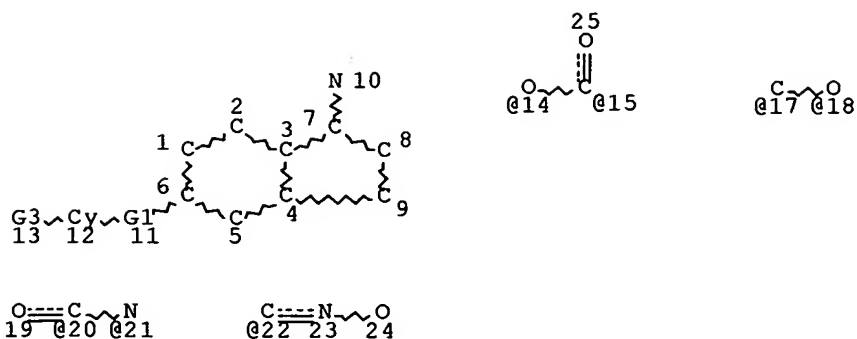
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 DEFAULT ECLEVEL IS LIMITED

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STEREO ATTRIBUTES: NONE  
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 L3 STR



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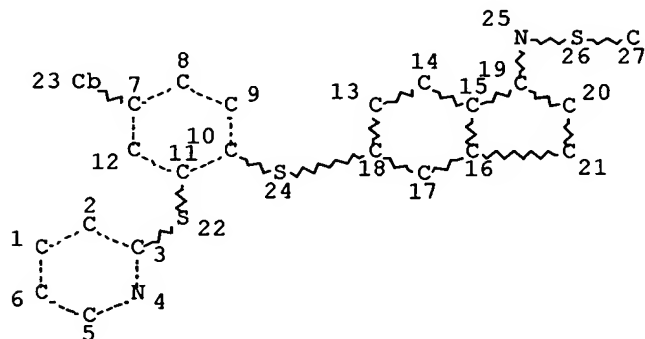
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 NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L4 207 SEA FILE=REGISTRY SUB=L2 SSS FUL L3  
 L15 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

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 L18 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L17  
 L19 205 SEA FILE=REGISTRY ABB=ON PLU=ON L4 NOT L17  
 L20 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L19  
 L21 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 NOT L18  
 L22 24 SEA FILE=HCAPLUS ABB=ON PLU=ON "TONG LING"/AU  
 L23 23 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 NOT (L18 OR L21)



L24 30 SEA FILE=HCAPLUS ABB=ON PLU=ON (("SHANKAR B"/AU OR "SHANKAR B B"/AU) OR ("SHANKAR BANDARPALLE"/AU OR "SHANKAR BANDARPALLE B"/AU OR "SHANKAR BANDERPALLE B"/AU)) NOT (L18 OR L21 OR L23)

L25 104 SEA FILE=HCAPLUS ABB=ON PLU=ON (("KOZLOWSKI J"/AU OR "KOZLOWSKI J A"/AU) OR ("KOZLOWSKI JOSEPH"/AU OR "KOZLOWSKI JOSEPH A"/AU OR "KOZLOWSKI JOSEPH ANDREW"/AU)) NOT (L18 OR L21 OR L23 OR L24)

L26 105 SEA FILE=HCAPLUS ABB=ON PLU=ON ("SHIH N"/AU OR "SHIH N Y"/AU OR ("SHIH NENG Y"/AU OR "SHIH NENG YANG"/AU)) NOT (L18 OR L21 OR L23 OR L24)

L27 2852 SEA FILE=HCAPLUS ABB=ON PLU=ON ("CHEN L"/AU OR "CHEN L A"/AU OR "CHEN L ALEX"/AU OR "CHEN L B"/AU OR "CHEN L BO"/AU OR "CHEN L C"/AU OR "CHEN L C L"/AU OR "CHEN L C M"/AU OR "CHEN L CHARLIE"/AU OR "CHEN L CHUN"/AU OR "CHEN L D"/AU OR "CHEN L E"/AU OR "CHEN L F"/AU OR "CHEN L F O"/AU OR "CHEN L G"/AU OR "CHEN L H"/AU OR "CHEN L H K"/AU OR "CHEN L I"/AU OR "CHEN L J"/AU OR "CHEN L JENNY"/AU OR "CHEN L K"/AU OR "CHEN L L"/AU OR "CHEN L M"/AU OR "CHEN L MICHAEL"/AU OR "CHEN L N"/AU OR "CHEN L P"/AU OR "CHEN L Q"/AU OR "CHEN L R"/AU OR "CHEN L S"/AU OR "CHEN L T"/AU OR "CHEN L W"/AU OR "CHEN L W A"/AU OR "CHEN L W ANTONY"/AU OR "CHEN L X"/AU OR "CHEN L X Q"/AU OR "CHEN L Y"/AU OR "CHEN L Z"/AU OR "CHEN L ZHONG"/AU) OR CHEN LEI ?/AU

L28 0 SEA FILE=HCAPLUS ABB=ON PLU=ON L25 AND L26 AND L27

L29 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L25 AND (L26 OR L27)

L30 0 SEA FILE=HCAPLUS ABB=ON PLU=ON L26 AND L27

L31 2 SEA FILE=HCAPLUS ABB=ON PLU=ON (L25 OR L26 OR L27) AND CANNABI?

L32 45 SEA FILE=HCAPLUS ABB=ON PLU=ON (L25 OR L26 OR L27) AND LIGAND

L33 50 SEA FILE=HCAPLUS ABB=ON PLU=ON L28 OR L29 OR L30 OR L31 OR L32

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L33 ANSWER 1 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:1331127 HCAPLUS Full-text  
 TITLE: Preparation of tartaric acid functional compounds for the treatment of inflammatory disorders  
 INVENTOR(S): Guo, Zhuyan; Orth, Peter; Zhu, Zhaoning; Mazzola, Robert D.; Chan, Tin Yau; Vaccaro, Henry A.; McKittrick, Brian; **Kozlowski, Joseph A.**; Lavey, Brian J.; Zhou, Guowei; Paliwal, Sunil; Wong, Shing-Chun; **Shih, Neng-Yang**; Ting, Pauline C.; Rosner, Kristin E.; Shipps, Gerald W. Jr.; Siddiqui, M. Arshad; Belanger, David B.; Dai, Chaoyang; Li, Dansu; Girijavallabhan, Vinay M.; Popovici-Muller, Janeta; Yu, Wensheng; Zhao, Lianyun  
 PATENT ASSIGNEE(S): Schering Corporation, USA  
 SOURCE: PCT Int. Appl., 889 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005121130	A2	20051222	WO 2005-US19131	20050601

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

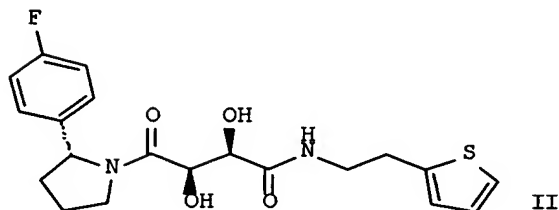
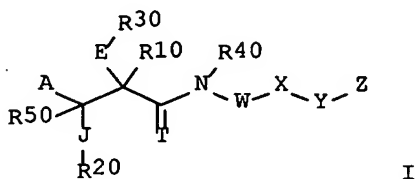
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PRIORITY APPLN. INFO.:

US 2004-576153P

P 20040602

GI



AB The title compds. I [A = (un)substituted benzimidazol-2-yl, imidazol-2-yl, CONH<sub>2</sub>, CSNH<sub>2</sub>; J, E = O, S, NR<sub>5</sub> (wherein R<sub>5</sub> = H, alkyl, alkylaryl); T = O, S; R<sub>10</sub>, R<sub>20</sub> = H, alkyl, fluoroalkyl; R<sub>30</sub> = H, alkyl or R<sub>30</sub> and R<sub>40</sub>, taken together with N to which R<sub>40</sub> is attached, are joined to form 4-7 membered (un)substituted heterocyclyl; R<sub>40</sub>, R<sub>50</sub> = H, alkyl; W = [C(R<sub>13</sub>)<sub>2</sub>]<sub>n</sub> (wherein n = 0-5; R<sub>13</sub> = H, halo, OH, etc.); X = a bond, alkyl, cycloalkyl, etc.; Y = a bond, O, S, NH, etc.; Z = H, alkyl, aryl, etc.; or their pharmaceutically acceptable salts] which can be useful for the treatment of diseases or conditions mediated by MMPs, ADAMs, TACE, TNF- $\alpha$  or combinations thereof, were prepared E.g., a multi-step synthesis of II, starting from 2,2-dimethyl-[1,3]dioxolane-4R,5R-dicarboxylic acid monomethyl ester and 2-(thien-1-yl)ethylamine, was given. The compds. I were tested against TACE (biol. data given for representative compds. I).

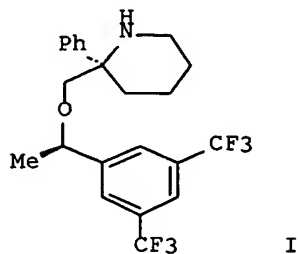
L33 ANSWER 2 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2005:1047070 HCAPLUS Full-text

DOCUMENT NUMBER: 143:477825

TITLE: Selective benzylic lithiation of N-Boc-2-phenylpiperidine and pyrrolidine: expedient synthesis of a 2,2-disubstituted piperidine NK1 antagonist

AUTHOR(S): Xiao, Dong; Lavey, Brian J.; Palani, Anandan; Wang, Cheng; Aslanian, Robert G.; Kozlowski, Joseph A.; Shih, Neng-Yang; McPhail, Andrew T.; Randolph, Gerard P.; Lachowicz, Jean E.; Duffy,

Ruth A.  
 CORPORATE SOURCE: Department of Chemical Research, Schering-Plough  
 Research Institute, Kenilworth, NJ, 07033, USA  
 SOURCE: Tetrahedron Letters (2005), 46(44), 7653-7656  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Unlike the lithiation of N-Boc-2-alkylpiperidines, which occurs at the 6-position, N-Boc-2-phenylpiperidine and N-Boc-2-phenylpyrrolidine can be lithiated exclusively at the 2-position. The tertiary carbanions can be trapped with a variety of electrophiles. This chemical was used for the synthesis of the potent NK1 **ligand I** ( $K_i = 0.3$  nM). The bioactive configuration at the piperidine quaternary center was determined by X-ray anal. to be (S).

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 3 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:952350 HCAPLUS Full-text

TITLE: Syntheses, properties and crystal structures of one-dimensional transition metal-azide coordination polymers via hydrogen bonds

AUTHOR(S): Li, Q.; Zhang, L.; Peng, F.; He, Y. Y.; Chen, L.; Tang, L. F.

CORPORATE SOURCE: Department of Chemical Engineering, Guangdong Provincial Laboratory for Green Chemical Technology, South China University of Technology, Guangzhou, 510640, Peop. Rep. China

SOURCE: Polish Journal of Chemistry (2005), 79(8), 1389-1397  
 CODEN: PJCHDQ; ISSN: 0137-5083

PUBLISHER: Polish Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three novel mononuclear transition metal azide compds.,  $Mn(PzBu-t)_4(N_3)_2$  (1),  $Co(PzBu-t)_4(N_3)_2$  (2) and  $Co(PzBu-t)_3(N_3)_3$  (3) ( $PzBu-t = 3$ -tert-butylpyrazole), have been synthesized and characterized by elemental anal., IR and UV-Vis spectra, and the crystal structures of compds. 1 and 3 have been determined. Crystal data for 1: triclinic, space group  $P\bar{1}$  with  $a = 8.0844(9)$ ,  $b = 10.1230(12)$ ,  $c = 12.1046(13)$  Å,  $\alpha = 91.854(3)^\circ$ ,  $\beta = 108.495(2)^\circ$ ,  $\gamma = 101.598(2)^\circ$ ,  $V = 915.33(18)$  Å<sup>3</sup> and  $Z = 1$ . Crystal data for 3: monoclinic,

space group P2(1) with  $a = 10.3286(9)$ ,  $b = 23.593(2)$ ,  $c = 12.7735(10)$  Å,  $\beta = 106.659(2)^\circ$ ,  $V = 2982.0(4)$  Å<sup>3</sup> and  $Z = 2$ . The azide ions in compound 1 are coordinated to manganese(II) ions in a trans centrosym. octahedral configuration. However, compound 3 shows two unsym. mols. with distorted octahedral geometry ligated by three azide anions and three 3-tert-butylpyrazole **ligands** in the crystal cell. The compds. are aggregated to form a one-dimensional chain through (pyrazole)N-H...N(azide) hydrogen bonds. In aqueous solution the reaction of compound 2 with azide (2 equiv) and H<sub>2</sub>O<sub>2</sub> was investigated and the product was isolated and identified as compound 3. This result suggests that compound 3, as the oxidation product of compound 2, was formed by the change of the coordination geometry around the cobalt ion due to the binding of peroxides to the cobalt ion during the removal of the pyrazole **ligand**.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 4 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:739804 HCAPLUS Full-text

TITLE: Discovery of novel hydroxamates as highly potent and selective TACE inhibitors: Part II - SAR development of mode A inhibitors

AUTHOR(S): Zhu, Z.; Mazzola, Robert; Sinning, Lisa; Lavey, Brian; Zhou, Guowei; Spitler, James; Wong, Shing-Chun; Orth, Peter; Guo, Zhuyan; Kong, Jianshe; Liang, Xian; Wong, Jesse; **Kozlowski, Joseph**; McKittrick, B.; **Shih, Neng-Yang**; Sun, Jing; Chen, Shu-Cheng; Niu, Xiao-Da; Sullivan, Lee; Lundell, Daniel

CORPORATE SOURCE: Chemical Research, Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Abstracts of Papers, 230th ACS National Meeting, Washington, DC, United States, Aug. 28-Sept. 1, 2005 (2005), MEDI-293. American Chemical Society: Washington, D. C.  
CODEN: 69HFCL

DOCUMENT TYPE: Conference; Meeting Abstract; (computer optical disk)

LANGUAGE: English

AB Through a de novo design approach, a potent Tumor Necrosis Factor - alpha (TNF-alpha) inhibitor based on a trans-cyclopropyldicarboxylate scaffold was identified. A focused SAR development effort was launched to optimize the enzyme binding affinity, selectivity against other MMPs and ADAMs, and pharmacokinetic profile which led to the discovery of Sch-7091456; an orally active TACE inhibitor (Fig. 1). Detailed SAR information and biol. data will be discussed in the presentation.

L33 ANSWER 5 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:705485 HCAPLUS Full-text

DOCUMENT NUMBER: 143:206680

TITLE: Endogenous release and multiple actions of secretin in the rat cerebellum

AUTHOR(S): Lee, S. M. Y.; **Chen, L.**; Chow, B. K. C.; Yung, W. H.

CORPORATE SOURCE: Department of Zoology, The University of Hong Kong, Pokfulam, Hong Kong, Peop. Rep. China

SOURCE: Neuroscience (Oxford, United Kingdom) (2005), 134(2), 377-386

CODEN: NRSCDN; ISSN: 0306-4522

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Previous studies demonstrated that secretin could modulate synaptic transmission in the rat cerebellum. In the present report, we provide evidence for the endogenous release of secretin in the cerebellum and further characterize the actions of secretin in this brain area. First, to show that secretin is released endogenously, blocks of freshly dissected cerebellum were challenged with a high concentration of KCl. Incubation with KCl almost doubled the rate of secretin release. This KCl-induced release was sensitive to tetrodotoxin and cadmium suggesting the involvement of voltage-gated sodium and calcium channels. The use of specific channel blockers further revealed that L-type and P/Q-type calcium channels underlie both basal and KCl-evoked secretin release. In support of this, depolarization of Purkinje neurons in the presence of NMDA, group II mGluR and **cannabinoid** CB1 receptor blockers resulted in increased inhibitory postsynaptic current frequency. Second, we found that the previously reported facilitatory action of secretin on GABAergic inputs to Purkinje neurons is partly dependent on the release of endogenous glutamate. In the presence of CNQX, an AMPA/kainate receptor antagonist, the facilitatory effect of secretin on GABA release was significantly reduced. In support of this idea, application of AMPA, but not kainate receptor agonist, facilitated GABA release from inhibitory terminals, an action that was sensitive to AMPA receptor antagonists. These data indicate that a direct and an indirect pathway mediate the action of secretin in the basket cell-Purkinje neuron synapse. The results provide further and more solid evidence for the role of secretin as a neuropeptide in the mammalian CNS.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 6 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:697592 HCAPLUS Full-text

TITLE: Crystal structure of bis[(1,10-phenanthroline-N,N')(2-bromobenzoato)-bis( $\mu$ -2-bromobenzoato)holmium(III)], [Ho(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)(BrC<sub>7</sub>H<sub>4</sub>O<sub>2</sub>)<sub>3</sub>]<sub>2</sub>

AUTHOR(S): Zhang, B.-S.; Zhu, X.-C.; Yu, Y.-Y.; **Chen, L.**; Chen, Z.-B.; Hu, Y.-M.

CORPORATE SOURCE: Normal College, Jinhua University, Zhejiang, 321017, Peop. Rep. China

SOURCE: Zeitschrift fuer Kristallographie - New Crystal Structures (2005), 220(2), 211-212  
CODEN: ZKNSFT; ISSN: 1433-7266

PUBLISHER: Oldenbourg Wissenschaftsverlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Crystallog. data and atomic coordinates are given. Within the [Ho(BrC<sub>6</sub>H<sub>4</sub>COO)(phen)( $\mu$ -BrC<sub>6</sub>H<sub>4</sub>COO)<sub>4/2</sub>]<sub>2</sub> complex mols., the Ho atoms are each coordinated by two N atoms from one bidentately chelating phenanthroline **ligand** and six O atoms from five bromobenzoic acid anions **ligands**, to complete a significantly distorted HoN<sub>2</sub>O<sub>6</sub> polyhedron environment with d(Ho-N) = 2.515(6) Å and 2.555(7) Å, d(Ho-O) = 2.249(6) - 2.437(5) Å. Four carboxy groups of bromobenzoic acid anions bridge Ho and Ho' atoms to a dinuclear complex. Moreover, the dinuclear mols. are connected to each other via weak hydrogen bonds between the bromobenzoic acid anion O atoms and phenanthroline C atoms. Through the weak hydrogen interactions the compound is interlinked to forms the 1D supramol. chains along the [010] direction.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 7 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

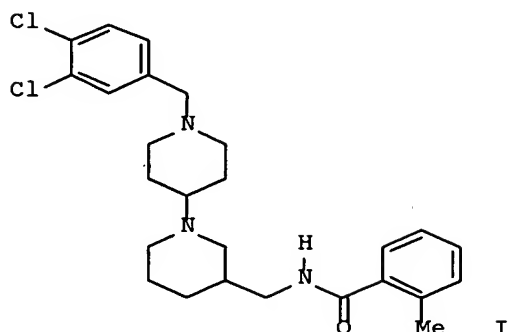
ACCESSION NUMBER: 2005:511367 HCAPLUS Full-text

DOCUMENT NUMBER: 143:172732

TITLE: The synthesis of substituted bipiperidine amide

compounds as CCR3 **ligands**: Antagonists  
versus agonists

AUTHOR(S): Ting, Pauline C.; Umland, Shelby P.; Aslanian, Robert;  
Cao, Jianhua; Garlisi, Charles G.; Huang, Ying;  
Jakway, James; Liu, Zhidan; Shah, Himanshu; Tian,  
Fang; Wan, Yuntao; **Shih, Neng-Yang**  
CORPORATE SOURCE: Schering Plough Research Institute, Kenilworth, NJ,  
07033, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),  
15(12), 3020-3023  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Structure-activity relationship study of bipiperidine amide has identified the reverse bipiperidine amide I as a CC chemokine-3 (CCR3) receptor antagonist. Optimization of the structure-activity relationship of I has resulted in the identification of a CCR3 antagonist as well as a CCR3 agonist.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 8 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:487333 HCAPLUS Full-text

DOCUMENT NUMBER: 143:129163

TITLE: Biological sensing with magnetic nanoparticles using Brownian relaxation (invited)

AUTHOR(S): Chung, S.-H.; Hoffmann, A.; Gusliencko, K.; Bader, S. D.; Liu, C.; Kay, B.; Makowski, L.; **Chen, L.**

CORPORATE SOURCE: Materials Science Division, Argonne National Laboratory, Argonne, IL, 60439, USA

SOURCE: Journal of Applied Physics (2005), 97(10, Pt. 3), 10R101/1-10R101/5

CODEN: JAPIAU; ISSN: 0021-8979

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Magnetic nanoparticles coated with biochem. **ligands** are enabling many biol. and medical applications. In particular biomagnetic sensors have potential advantages of simplicity and rapidity. The authors demonstrate a substrate-

free biomagnetic sensing approach using the magnetic a.c. susceptibility of ferromagnetic particles suspended in a liquid. The magnetic relaxation of these particles is mainly due to Brownian rotational diffusion, which can be modified by binding the particles to the intended target. This scheme has several advantages: (i) it requires only one binding event; (ii) there is an inherent check of integrity; and (iii) the signal contains addnl. information about the target size.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 9 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:476989 HCAPLUS Full-text

TITLE: Capturing excited state molecular structures in disordered media with 100 ps time resolution by laser pump X-ray probe XAFS

AUTHOR(S): Chen, L. X.; Shaw, G. B.; Liu, T.; Jennings, G.; Attenkofer, K.

CORPORATE SOURCE: Chemistry Division, Argonne National Laboratory  
Argonne, IL, 60439, USA

SOURCE: Physica Scripta, T (2005), T115(12th X-Ray Absorption Fine Structure International Conference (XAFS12), 2003), 93-96

CODEN: PHSTER; ISSN: 0281-1847

PUBLISHER: Royal Swedish Academy of Sciences

DOCUMENT TYPE: Journal; (computer optical disk)

LANGUAGE: English

AB The timing structure and the high photon flux of X-ray pulses from the Advanced Photon Source permit pump-probe techniques widely used in ultrafast laser spectroscopy to be extended into the X-ray regime. The intrinsic time resolution of the expts. is determined by the FWHM of the single pulses from the synchrotron at 70-100 ps. The challenges and the solns. in such expts. will be discussed. Using laser pulse pump, X-ray pulse probe XAFS, several excited state mol. structures in solns. were studied. We will mainly describe mol. structures of the photoexcited metal-to-ligand-charge-transfer state of [CuI(dmp)2]<sup>+</sup>, where dmp is 2,9-dimethyl-1,10-phenanthroline, in toluene and acetonitrile. The exptl. results indicated that the copper ion in the thermally equilibrated MLCT state in both solvents had the same oxidation state as the corresponding Cu(II) complex in the ground state and was found to be penta-coordinate with an average nearest neighbor Cu-N distances 0.04 Å longer in toluene and 0.04 Å shorter in acetonitrile than that of the ground state [CuI(dmp)2]<sup>+</sup>. The results further revealed that what distinguishes the MLCT state structures in non-coordinating and coordinating solvents is not the "exciplex" formation, but the strength of the interactions between the solvent and the Cu(II)\* species at the MLCT state. In addition, future direction of time-resolved XAFS will be discussed.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 10 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:289004 HCAPLUS Full-text

DOCUMENT NUMBER: 142:367948

TITLE: Enhanced striatal opioid receptor-mediated G-protein activation in L-dopa-treated dyskinetic monkeys

AUTHOR(S): Chen, L.; Togasaki, D. M.; Langston, J. W.; Di Monte, D. A.; Quik, M.

CORPORATE SOURCE: Basic Research Department, The Parkinson's Institute, Sunnyvale, CA, 94089, USA

SOURCE: Neuroscience (Oxford, United Kingdom) (2005), 132(2), 409-420

CODEN: NRSCDN; ISSN: 0306-4522

PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Long-term L-3,4-dihydroxyphenylalanine (L-dopa) treatment in Parkinson's disease leads to dyskinesias in the majority of patients. The underlying mol. mechanisms for L-dopa-induced dyskinesias (LIDs) are currently unclear. However, the findings that there are alterations in opioid peptide mRNA and protein expression and that opioid ligands modulate dyskinesias suggest that the opioid system may be involved. To further understand its role in dyskinesias, we mapped opioid receptor-stimulated G-protein activation using [35S]guanylyl-5'-O-( $\gamma$ -thio)-triphosphate ([35S]GTP $\gamma$ S) autoradiog. in the basal ganglia of normal and 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP)-lesioned squirrel monkeys administered water or L-dopa. Subtype-selective opioid receptor G-protein coupling was investigated using the  $\mu$ -opioid agonist [D-Ala,N-Me-Phe,Gly-ol]-enkephalin,  $\delta$ -agonist SNC 80 and  $\kappa$ -agonist U 50488H. Our data show that  $\mu$ -opioid receptor-mediated G-protein activation is significantly enhanced in the basal ganglia and cortex of L-dopa-treated dyskinetic monkeys, whereas  $\delta$ - and  $\kappa$ -receptor-induced increases were limited to only a few regions. A similar pattern of enhancement was observed in both MPTP-lesioned and unlesioned animals with LIDs suggesting the effect was not simply due to a compromised nigrostriatal system. Opioid receptor G-protein coupling was not enhanced in non-dyskinetic L-dopa-treated animals, or lesioned monkeys not given L-dopa. The increases in opioid-stimulated [35S]GTP $\gamma$ S binding are directly correlated with dyskinesias. The present data demonstrate an enhanced subtype-selective opioid-receptor G-protein coupling in the basal ganglia of monkeys with LIDs. The pos. correlation with LIDs suggests this may represent an intracellular signaling mechanism underlying these movement abnormalities.

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 11 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:128404 HCAPLUS Full-text

DOCUMENT NUMBER: 142:367972

TITLE: Expression and spatial distribution of secretin and secretin receptor in human cerebellum

AUTHOR(S): Lee, S. M. Y.; Yung, W. H.; **Chen, L.**; Chow, B. K. C.

CORPORATE SOURCE: Department of Zoology, Faculty of Science, The University of Hong Kong, Pokfulam, Hong Kong

SOURCE: NeuroReport (2005), 16(3), 219-222  
 CODEN: NERPEZ; ISSN: 0959-4965

PUBLISHER: Lippincott Williams & Wilkins

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The expression and spatial distribution of secretin and its receptor in human cerebellum were investigated by in situ hybridization and immunohistochem. techniques. Secretin mRNAs are found in Purkinje cells, whereas secretin receptor transcripts are present in Purkinje cells and basket cells in the mol. cell layer. In addition, secretin-immunoreactivities are localized in both the soma and dendrites of Purkinje cells. These data are the first demonstration of the spatial distribution of secretin and its receptor in distinct neurons within the human cerebellum. The cellular localizations of this ligand-receptor pair are consistent with the proposed actions of secretin in the cerebellum of rodents and hence suggest that secretin also serves specific neural functions in the human cerebellum.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L33 ANSWER 12 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:74703 HCAPLUS Full-text

DOCUMENT NUMBER: 142:211436

TITLE: Triaryl bis-sulfones as a new class of **cannabinoid** CB2 receptor inhibitors: identification of a lead and initial SAR studies

AUTHOR(S): Lavey, Brian J.; Kozlowski, Joseph A.; Hipkin, R. William; Gonsiorek, Waldemar; Lundell, Daniel J.; Piwinski, John J.; Narula, Satwant; Lunn, Charles A.

CORPORATE SOURCE: Department of Chemistry, Schering-Plough Research Institute, Kenilworth, NJ, 07033-0539, USA

SOURCE: Bioorganic &amp; Medicinal Chemistry Letters (2005), 15(3), 783-786

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:211436

AB A novel class of **cannabinoid** CB2 receptor **ligands** is described. These triaryl bis-sulfones are nanomolar inhibitors of the CB2 receptor and show high selectivity over the **cannabinoid** CB1 receptor. One example of this new class decreases **ligand**-induced GTP $\gamma$ S binding to recombinant CB2 cell membranes, identifying the compound as a CB2-selective inverse agonist.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 13 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:558763 HCAPLUS Full-text

DOCUMENT NUMBER: 141:348438

TITLE: Expression of TRAIL, DR4, and DR5 in kidney and serum from patients receiving renal transplantation

AUTHOR(S): Song, C. J.; Liu, X. S.; Zhu, Y.; Chen, L. H.; Jia, W.; Li, Y. N.; Cao, Y. X.; Xie, X.; Zhuang, R.; Zhu, C. S.; Jin, B. Q.

CORPORATE SOURCE: Department of Immunology, Fourth Military Medical University, Xi'an, Peop. Rep. China

SOURCE: Transplantation Proceedings (2004), 36(5), 1340-1343

CODEN: TRPPA8; ISSN: 0041-1345

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Renal transplantation is the best treatment of some end-stage renal diseases. Unfortunately, not every transplant is successful due to the rejection or dysfunction of the transplanted kidney. Many cytokines participate in rejection by inducing inflammation or apoptosis. In this study, the expressions of TRAIL, DR4, and DR5 in rejected renal tissue and of serum soluble TRAIL (sTRAIL) in patients with kidney rejection were investigated by immunohistochem. staining and sandwich ELISA, resp. The results showed that the expression of TRAIL, DR4 and DR5, and serum sTRAIL levels were markedly upregulated among renal transplant patients. Since both membrane and soluble forms of TRAIL can induce apoptosis of DR4/DR5-expressing cells via recruiting FADD and caspase 8, elevated TRAIL and its receptors may participate in renal graft rejection.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 14 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:345455 HCAPLUS Full-text

DOCUMENT NUMBER: 141:116233

TITLE: Gastrointestinal stromal tumors: overview of pathologic features, molecular biology, and therapy with imatinib mesylate

AUTHOR(S): Koh, J. S.; Trent, J.; **Chen, L.**; El-Naggar, A.; Hunt, K.; Pollock, R.; Zhang, W.

CORPORATE SOURCE: Departments of Pathology, Sarcoma Oncology, and Surgical Oncology, The University of Texas M.D. Anderson Cancer Center, Houston, TX, USA

SOURCE: Histology and Histopathology (2004), 19(2), 565-574  
CODEN: HIHIES; ISSN: 0213-3911

PUBLISHER: Jimenez Godoy, S.A.

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. Gastrointestinal stromal tumors (GISTs) are the most common mesenchymal tumors of the gastrointestinal tract. These tumors develop at any site but are most commonly reported in the stomach. They originate from the neoplastic transformation of the intestinal pacemaker cell, the interstitial cell of Cajal. GISTs strongly express the receptor tyrosine kinase KIT and have mutations in the KIT gene, most frequently in exon 11 encoding the intracellular juxtamembranous region. Expression of KIT is seen in almost all GISTs, and is thus regarded as one of the key diagnostic markers. Distinction from smooth muscle tumors, such as leiomyosarcomas, and other mesenchymal tumors is very important because of prognostic differences and therapeutic strategies. Predicting the biol. behavior of GISTs is often difficult by conventional pathol. examination; tumor size and mitotic rate are the most important prognostic indicators. The prognostic significance of KIT mutations is controversial and thus far has not been clearly linked with biol. behavior. KIT mutations are associated with tumor development, and cytogenetic aberrations are associated with tumor progression. The pathogenesis of GISTs involves a gain-of-function mutation in the KIT proto-oncogene, leading to **ligand** -independent constitutive activation of the KIT receptor. KIT-wild-type GISTs have shown mutually exclusive platelet-derived growth factor receptor (PDGFR) mutation and activation. The use of imatinib mesylate (also known as Gleevec or STI-571) has greatly increased the therapeutic efficacy for this otherwise chemotherapy-resistant tumor. GISTs with very low levels of KIT expression may respond to imatinib mesylate therapy if the receptors are activated by specific mechanisms. KIT-activating mutations fall into 2 groups: the regulatory type and the enzymic site type. The regulatory type of mutation is conserved at the imatinib binding site, whereas the enzymic site mutation has a structurally changed drug-binding site, resulting in drug resistance. The authors summarize the pathol. features of GISTs, recent advances in understanding their mol. and biol. features, and therapy with imatinib mesylate.

REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 15 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:855801 HCAPLUS Full-text

DOCUMENT NUMBER: 139:350734

TITLE: Preparation of 1-(4-piperidinyl)benzimidazoles as histamine H3 antagonists

INVENTOR(S): Zeng, Qingbei; Aslanian, Robert G.; Berlin, Michael Y.; Boyce, Christopher W.; Cao, Jianhua;  
**Kozlowski, Joseph A.**; Mangiaracina, Pietro;  
McCormick, Kevin D.; Mutahi, Mwangi W.; Rosenblum, Stuart B.; **Shih, Neng-Yang**; Solomon, Daniel M.; Tom, Wing C.

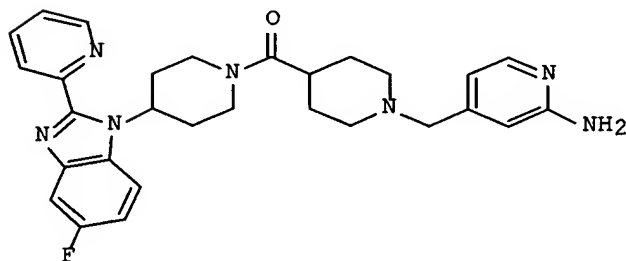
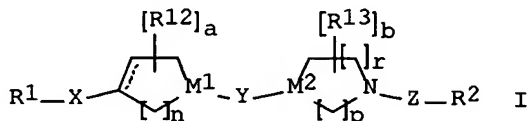
PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 132 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003088967	A1	20031030	WO 2003-US11672	20030416
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2481940	AA	20031030	CA 2003-2481940	20030416
US 2004097483	A1	20040520	US 2003-417391	20030416
EP 1499316	A1	20050126	EP 2003-719766	20030416
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003009348	A	20050301	BR 2003-9348	20030416
JP 2005529116	T2	20050929	JP 2003-585719	20030416
NO 2004005002	A	20050118	NO 2004-5002	20041117
PRIORITY APPLN. INFO.:			US 2002-373731P	P 20020418
			US 2002-373467P	P 20020418
			WO 2003-US11672	W 20030416

OTHER SOURCE(S): MARPAT 139:350734  
 GI



AB The title compds. [I; R1 = (un)substituted benzimidazolyl or a derivative thereof; R2 = (un)substituted aryl or heteroaryl; M1, M2 = CR3, N; X = a bond, alkylene; Y = CO, CS, SO2, etc.; Z = a bond, alkylene, CO, etc.; R3 = H, halo, alkyl, etc.; R12 = alkyl, OH, alkoxy, etc.; R13 = alkyl, alkoxy, OH, etc.; a, b = 0-2; n, p = 1-3; r = 0-3; with the provisos] which are histamine H3 antagonists, were prepared E.g., a multi-step synthesis of II which showed Ki of 1 nM in rHu H3 binding assay, was given. Also disclosed are pharmaceutical

comps. comprising the compds. of formula I and methods of treating various diseases or conditions, such as allergy, allergy-induced airway responses, and congestion (e.g., nasal congestion) using the compds. I. Also disclosed are methods of treating said diseases or conditions using the compds. of formula I in combination with an H1 receptor antagonist.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 16 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:621826 HCAPLUS Full-text

DOCUMENT NUMBER: 139:305771

TITLE: The fragile X mental retardation protein binds and regulates a novel class of mRNAs containing U rich target sequences

AUTHOR(S): **Chen, L.**; Yun, S.-W.; Seto, J.; Liu, W.; Toth, M.

CORPORATE SOURCE: Weill Medical College, Department of Pharmacology, Cornell University, New York, NY, 10021, USA

SOURCE: Neuroscience (Oxford, United Kingdom) (2003), 120(4), 1005-1017

CODEN: NRSCDN; ISSN: 0306-4522

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fragile X syndrome is a common form of inherited mental retardation caused by the absence of the fragile X mental retardation protein (FMRP). It has been hypothesized that FMRP is involved in the processing and/or translation of mRNAs. Human and mouse target-mRNAs, containing purine quartets, have previously been identified. By using cDNA-SELEX (systematic evolution of **ligands** by exponential enrichment), we identified another class of human target-mRNAs which contain U rich sequences. This technique, in contrast to oligonucleotide-based SELEX, allows the identification of FMRP targets directly from mRNA pools. Many of the proteins encoded by the identified FMRP targets have been implicated in neuroplasticity. Steady state levels of target-mRNAs were unchanged in the brain of fragile X mice. However, levels of two target-encoded proteins, an L-type calcium channel subunit and MAP1B, were downregulated in specific brain regions suggesting a defect in the expression of target-encoded proteins in fragile X syndrome.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 17 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:511283 HCAPLUS Full-text

DOCUMENT NUMBER: 139:85038

TITLE: Preparation of TNF- $\alpha$  inhibiting hydroxyamic or carboxylic acid functionalized cycloalkanes for the treatment of inflammatory disorders

INVENTOR(S): Zhu, Zhaoning; Mazzola, Robert, Jr.; Guo, Zhuyan; Lavey, Brian J.; Sinning, Lisa; **Kozlowski, Joseph**; McKittrick, Brian; **Shih, Neng-Yang**

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 179 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

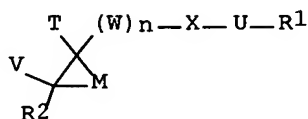
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

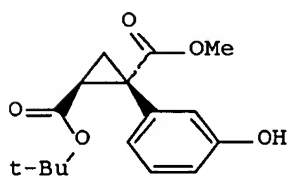
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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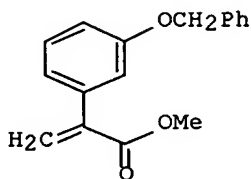
WO 2003053915	A2	20030703	WO 2002-US40453	20021219
WO 2003053915	A3	20030918		
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CA 2470620	AA	20030703	CA 2002-2470620	20021219
US 2004038941	A1	20040226	US 2002-323511	20021219
US 6838466	B2	20050104		
EP 1458676	A2	20040922	EP 2002-792429	20021219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005513125	T2	20050512	JP 2003-554632	20021219
US 2004102418	A1	20040527	US 2003-716890	20031119
PRIORITY APPLN. INFO.:			US 2001-342332P	P 20011220
			US 2002-323511	A3 20021219
			WO 2002-US40453	W 20021219
OTHER SOURCE(S):			MARPAT 139:85038	
GI				



I



II



III

AB This invention relates to compds. of formula I [M = -(C(R30)(R40))<sub>m</sub>-, wherein m = 1-6; T = substituted alkyl, (un)substituted-cycloalkyl, -heterocycloalkyl, -aryl, etc.; V = (un)substituted alkyl, cycloalkyl, heteroaryl, etc.; R<sup>1</sup> = (un)substituted alkyl, alkyne, alkene, cycloalkyl, aryl, etc.; R<sup>2</sup> = H, halo, (un)substituted alkyl, cycloalkyl, etc.; U = bond, alkyl, heteroalkyl, heteroatoms; X = (un)substituted alkylene, cycloalkylene, arylene, etc.; W = carboxy, substituted iminomethylene, SO<sub>2</sub>, SO, etc., wherein n = 0-2; R<sub>30</sub> and R<sub>40</sub> independently = H or halo, CN, NO<sub>2</sub>, (un)substituted alkyl, etc.; or R<sub>30</sub> and R<sub>40</sub> may be taken together with the atom to which they are attached to form C=O, with provisions] or a pharmaceutically acceptable salt, solvate or isomer thereof, which can be useful for the treatment of diseases or conditions mediated by MMPs, TNF-alpha or combinations thereof. Thus, II was prepared from Me methoxyphenylethanoate with the cyclopropane ring diastereoselectively formed by cyclization of intermediate III with S-carbo-tert-

butoxymethyltetrahydrothiophene bromide with subsequent hydrogenation and resolution of enantiomers. Numerous compds. of the invention possessed  $K_i$  values of less than 20 nM in a TNF- $\alpha$  convertases (TACE) inhibitory activity assay. As TNF- $\alpha$  inhibitors, I will be useful in treatment of inflammatory disorders.

L33 ANSWER 18 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:420452 HCAPLUS Full-text

DOCUMENT NUMBER: 139:332653

TITLE: An assessment of the mechanistic differences between two integrin  $\alpha 4\beta 1$  inhibitors, the monoclonal antibody TA-2 and the small molecule BIO5192, in rat experimental autoimmune encephalomyelitis

AUTHOR(S): Leone, D. R.; Giza, K.; Gill, A.; Dolinski, B. M.; Yang, W.; Perper, S.; Scott, D. M.; Lee, W.-C.; Cornebise, M.; Wortham, K.; Nickerson-Nutter, C.; **Chen, L. L.**; Lepage, D.; Spell, J. C.; Whalley, E. T.; Petter, R. C.; Adams, S. P.; Lobb, R. R.; Pepinsky, R. B.

CORPORATE SOURCE: Biogen, Inc., Cambridge, MA, USA

SOURCE: Journal of Pharmacology and Experimental Therapeutics (2003), 305(3), 1150-1162

CODEN: JPETAB; ISSN: 0022-3565

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal

LANGUAGE: English

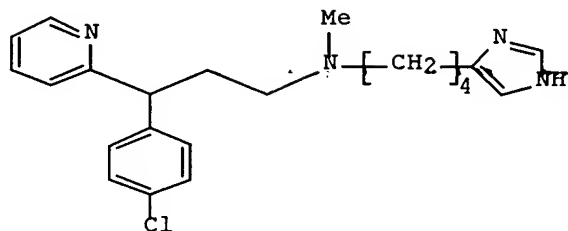
AB Integrin  $\alpha 4\beta 1$  plays an important role in inflammatory processes by regulating the migration of lymphocytes into inflamed tissues. Here we evaluated the biochem., pharmacol., and pharmacodynamic properties and efficacy in exptl. autoimmune encephalomyelitis (EAE), a model of multiple sclerosis, of two types of  $\alpha 4\beta 1$  inhibitors, the anti-rat  $\alpha 4$  monoclonal antibody TA-2 and the small mol. inhibitor BIO5192 [2(S)-{[1-(3,5-dichloro-benzenesulfonyl)-pyrrolidine-2(S)-carbonyl]-amino}-4-[4-methyl-2(S)-(methyl-[2-(4-(3-o-tolyl-ureido)-phenyl]-acetyl)-amino)-pentanoylamino]-butyric acid]. TA-2 has been extensively studied in rats and provides a benchmark for assessing function. BIO5192 is a highly selective and potent ( $K_D$  of  $<10$  pM) inhibitor of  $\alpha 4\beta 1$ . Dosing regimens were identified for both inhibitors, which provided full receptor occupancy during the duration of the study. Both inhibitors induced leukocytosis, an effect that was used as a pharmacodynamic marker of activity, and both were efficacious in the EAE model. Treatment with TA-2 caused a decrease in  $\alpha 4$  integrin expression on the cell surface, which resulted from internalization of  $\alpha 4$  integrin/TA-2 complexes. In contrast, BIO5192 did not modulate cell surface  $\alpha 4\beta 1$ . Our results with BIO5192 indicate that  $\alpha 4\beta 7$  does not play a role in this model and that blockade of  $\alpha 4\beta 1$ /ligand interactions without down-modulation is sufficient for efficacy in rat EAE. BIO5192 is highly selective and binds with high affinity to  $\alpha 4\beta 1$  from four of four species tested. These studies demonstrate that BIO5192, a novel, potent, and selective inhibitor of  $\alpha 4\beta 1$  integrin, will be a valuable reagent for assessing  $\alpha 4\beta 1$  biol. and may provide a new therapeutic for treatment of human inflammatory diseases.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 19 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:405927 HCAPLUS Full-text

DOCUMENT NUMBER: 139:190628  
 TITLE: Identification of a dual histamine H1/H3 receptor **ligand** based on the H1 antagonist chlorpheniramine  
 AUTHOR(S): Aslanian, Robert; Mutahi, Mwangi Wa; **Shih, Neng-Yang**; Piwinski, John J.; West, Robert; Williams, Shirley M.; She, Susan; Wu, Ren-Long; Hey, John A.  
 CORPORATE SOURCE: The Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(12), 1959-1961  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:190628  
 GI



AB Combining the first generation H1 antihistamine chlorpheniramine with H3 **ligands** of the alkylamine type has led to the identification of compound (I) a dual **ligand** of both the H1 and H3 receptors.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 20 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:691693 HCAPLUS Full-text

DOCUMENT NUMBER: 137:358606

TITLE: Surface Restructuring of Nanoparticles: An Efficient Route for **Ligand**-Metal Oxide Crosstalk

AUTHOR(S): Rajh, T.; **Chen, L. X.**; Lukas, K.; Liu, T.; Thurnauer, M. C.; Tiede, D. M.

CORPORATE SOURCE: Chemistry Division, Argonne National Laboratory, Argonne, IL, 60439, USA

SOURCE: Journal of Physical Chemistry B (2002), 106(41), 10543-10552

CODEN: JPCBFK; ISSN: 1520-6106

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Surface modification of nanocryst. metal oxide particles with enediol **ligands** results in altered optical properties of nanoparticles. The surface modification results in a red shift of the semiconductor absorption compared to unmodified nanocrystallites. The optical shift is correlated to the dipole

moment of the Ti-ligand complexes at the particle surface and decreases with the ligand size. The binding is exclusively characteristic of colloids in the nanocryst. domain (<20 nm). X-ray near-edge structure measurements at Ti K edge indicate that in this size domain the surface Ti atoms adjust their coordination environment to form undercoordinated sites. These 5-coordinated defect sites are the source of novel enhanced and selective reactivity of the nanoparticle toward bidentate ligand binding as observed using IR spectroscopy. Enediol ligands have the optimal geometry for chelating surface Ti atoms, resulting in a 5-membered ring coordination complex and restored 6-coordinated octahedral geometry of surface Ti atoms. The binding of enediol ligands is enhanced because of the stability gained from adsorption-induced restructuring of the nanoparticle surface. Consistent behavior was found for the 3 different nanocryst. metal oxide systems: TiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, and ZrO<sub>2</sub>.

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 21 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:136921 HCAPLUS Full-text

DOCUMENT NUMBER: 137:93725

TITLE: Synthesis and structure-Activity relationships of M2-Selective muscarinic receptor ligands in the 1-[4-(4-Arylsulfonyl)-phenylmethyl]-4-(4-piperidinyl)-piperazine family

AUTHOR(S): McCombie, Stuart W.; Lin, Sue-Ing; Tagat, Jayaram R.; Nazareno, Dennis; Vice, Susan; Ford, Jennifer; Asberom, Theodros; Leone, Daria; Kozlowski, Joseph A.; Zhou, Guowei; Ruperto, Vilma B.; Duffy, Ruth A.; Lachowicz, Jean E.

CORPORATE SOURCE: Department of Chemistry, Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(5), 795-798

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:93725

AB The synthesis and muscarinic binding properties of compds. based on the 1-[[4-(4-arylsulfonyl)phenyl]methyl]-4-(1-aroyl-4-piperidinyl)piperazine skeleton are described. For compds. substituted with appropriately configured Me groups at the benzylic center and at the piperazine 2-position, high levels of selective, M2 subtype affinity could be obtained, particularly when the terminal N-aroyl residue was ortho substituted.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 22 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:136920 HCAPLUS Full-text

DOCUMENT NUMBER: 137:103390

TITLE: Substituted 2-(R)-Methyl piperazines as muscarinic M2 selective ligands

AUTHOR(S): Kozlowski, Joseph A.; Zhou, Guowei; Tagat, Jayaram R.; Lin, Sue-Ing; McCombie, Stuart W.; Ruperto, Vilma B.; Duffy, Ruth A.; McQuade, Robert A.; Crosby, Gordon; Taylor, Lisa A.; Billard, William; Binch, Herbert; Lachowicz, Jean E.

CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ, 07033-0539, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(5), 791-794



CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:103390  
 AB A novel series of 2-(R)-methyl-substituted piperazines is described. They are potent M2 selective **ligands** that have >100-fold selectivity vs. the M1 receptor. In the rat microdialysis assay, one compound showed significantly enhanced levels of acetylcholine after oral administration.  
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 23 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2001:609536 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:268483  
 TITLE: Suppression of Fas **ligand** expression on endothelial cells by arsenite through reactive oxygen species  
 AUTHOR(S): Tsai, S.-H.; Hsieh, M.-S.; **Chen, L.**; Liang, Y.-C.; Lin, J.-K.; Lin, S.-Y.  
 CORPORATE SOURCE: Department of Orthopaedics and Traumatology, Taipei Medical University, School of Medicine, Taipei, Taiwan  
 SOURCE: Toxicology Letters (2001), 123(1), 11-19  
 CODEN: TOLED5; ISSN: 0378-4274  
 PUBLISHER: Elsevier Science Ireland Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Chronic exposure to arsenite is associated with vascular disease, such as arteriosclerosis. However, the cellular mechanisms for vascular disease in response to arsenic are not well known. The present study has demonstrated that arsenite not arsenate decreased the Fas **ligand** (FasL) expression on ECV304 cells through reactive oxygen species. Incubation of ECV304 cells with arsenite decreased the FasL expression and increased the intracellular peroxide levels. In addition, hydrogen peroxide was found to suppress FasL expression in a dose-dependent manner. The antioxidant, N-acetyl-cysteine, blocked the suppression of FasL expression in response to arsenite. These data suggested that arsenite initiates endothelium dysfunction, at least partly, by suppressing the FasL expression through activating reactive oxygen species sensitive endothelial cell signaling.  
 REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 24 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2001:518686 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:350381  
 TITLE: Probing transient molecular structures with time-resolved pump/probe XAFS using synchrotron x-ray sources  
 AUTHOR(S): **Chen, L. X.**  
 CORPORATE SOURCE: Chemistry Division, Argonne National Laboratory, Argonne, IL, 60439, USA  
 SOURCE: Journal of Electron Spectroscopy and Related Phenomena (2001), 119(2-3), 161-174  
 CODEN: JESRAW; ISSN: 0368-2048  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Laser pulse pump, x-ray pulse probe x-ray absorption fine structure (pump-probe XAFS) expts. using synchrotron sources are described from tech. considerations and from scientific significance. There are 3 tech. challenges

of such expts.: (1) laser photoexcitation, (2) synchronization of laser pulse and x-ray pulse, and (3) detection; each of which is studied. Based on the results the transient mol. structure of a reaction intermediate produced by photoexcitation of NiTPP-L2 (NiTPP, nickeltetraphenylporphyrin; L, piperidine) in solution was captured for the 1st time with the pump-probe XAFS on a 14-ns time scale obtained from the x-ray pulses from a 3rd generation synchrotron source. The exptl. results confirm that photoexcitation leads to the rapid removal of both axial ligands to produce a transient square-planar intermediate, NiTTP, with a lifetime of 28 ns. The transient structure of the photodissociated intermediate is nearly identical to that of the ground state NiTPP, suggesting that the intermediate adopts the same structure as the ground state in a noncoordinating solvent before it recombines with 2 ligands to form the more stable octahedrally coordinated NiTPP-L2. No detectable population of a pentacoordinated intermediate was present. This experiment demonstrates the feasibility of determining transient mol. structures in disordered media using the temporal resolution of a synchrotron x-ray source.

REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 25 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:428899 HCAPLUS Full-text

DOCUMENT NUMBER: 135:146793

TITLE: 3D QSAR analyses of novel tyrosine kinase inhibitors based on pharmacophore alignment

AUTHOR(S): Zhu, L. L.; Hou, T. J.; Chen, L. R.; Xu, X. J.

CORPORATE SOURCE: College of Chemistry and Molecular Engineering and Department of Technical Physics, Peking University, Beijing, 100871, Peop. Rep. China

SOURCE: Journal of Chemical Information and Computer Sciences (2001), 41(4), 1032-1040  
CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In an effort to develop a quant. ligand-binding model for the receptor tyrosine kinases, a pharmacophore search was first used to identify structural features that are common in two novel sets of 12 mols. of the 3-substituted indolin-2-ones and 19 compds. of the benzylidene malononitriles with low-to-high affinity for HER2, a kind of receptor tyrosine kinase. The common pharmacophore model based on these 31 compds. was used as a template to obtain the aligned mol. aggregate, which provided a good starting point for 3D-QSAR anal. of only the 19 benzylidene malononitriles. Two mol. field anal. (MFA) techniques, including CoMFA and CoMSIA, were used to derive the quant. structure-activity relationships of the studied mols. From the studied results, it was obvious that the 3D-QSAR models based on the pharmacophore alignment were superior to those based on the simple atom-by-atom fits. Considering the flexibility of the studied mols. and the difference between the active conformers and the energy-lowest conformers, the pharmacophore model can usually provide the common features for the flexible regions. Moreover, the best CoMSIA model based on the pharmacophore hypothesis gave good statistical measure from partial least-squares anal. (PLS) ( $q^2 = 0.71$ ), which was slightly better than the CoMFA one. Our study demonstrated that pharmacophore modeling and CoMSIA research could be effectively combined. Results obtained from both methods helped with understanding the specific activity of some compds. and designing new specific HER2 inhibitors.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 26 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:426308 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:235454  
 TITLE: Silver ion-selective electrodes based on novel  
 benzothiazolyl containing calix[4]arene  
 AUTHOR(S): **Chen, L.**; Ju, H.; Zeng, X.; He, X.; Zhang,  
 Z.  
 CORPORATE SOURCE: Department of Chemistry, Nankai University, Tianjin,  
 300071, Peop. Rep. China  
 SOURCE: Analytica Chimica Acta (2001), 437(2), 191-197  
 CODEN: ACACAM; ISSN: 0003-2670  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The Ag ion-selective electrodes (ISEs) were prepared by incorporating four novel calix[4]arene derivs. substituted by benzothiazolyl units, as the neutral carrier into the plasticized polymeric membranes. The construction, response characteristic and application of Ag ISEs were studied. The better results were obtained with membranes containing bis(2-benzothiazolyl) groups (**ligand** 1,2) with di-Bu phosphate (DBP) as a plasticizer. The electrodes show good Nernstian response to Ag<sup>+</sup> over a wide concentration range (5 + 10<sup>-6</sup>-1 + 10<sup>-1</sup> M) for electrodes based on calix[4]arene derivs. containing benzothiazolyl groups and excellent selectivity against alkali, alkaline earth and some transition metal ions. The electrode was used as indicator electrode in titration of Ag<sup>+</sup> with Cl<sup>-</sup> ions.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 27 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:99728 HCAPLUS Full-text  
 DOCUMENT NUMBER: 134:366451  
 TITLE: Kinetics and mechanism of carboxy ester hydrolysis  
 using Zn(II) complexes with functionalized  
 phenanthroline complexes  
 AUTHOR(S): Su, X.-C.; Sun, H.-W.; Zhou, Z.-F.; Lin, H.-K.;  
**Chen, L.**; Zhu, S.-R.; Chen, Y.-T.  
 CORPORATE SOURCE: Department of Chemistry, Nankai University, Tianjin,  
 300071, Peop. Rep. China  
 SOURCE: Polyhedron (2001), 20(1-2), 91-95  
 CODEN: PLYHDE; ISSN: 0277-5387  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Zn(II) complexes of six new functionalized phenanthrolines were examined as catalysts for the hydrolysis of 4-nitrophenyl acetate (NA). The new **ligands** form a 1:1 Zn complex in the pH range 6.5-9.0. In the kinetic studies using the Zn complexes in 10% (volume/volume) MeCN at 298 K, I = 0.10 mol dm<sup>-3</sup> KNO<sub>3</sub> and pH 6.8-9.0, it was shown than an axial OH<sup>-</sup> serves as a good nucleophile that effectively catalyzes NA hydrolysis. The hydrolysis rate follows the law  $v = (k_{\text{plus[complex]}} + k_{\text{OH[OH-]}} + k_{\text{co}})[\text{NA}]$ . The second-order rate consts. of ZnLH-1 are 0.934, 0.420, 0.360, 0.307, 0.257 and 0.143 mol<sup>-1</sup> dm<sup>3</sup> s<sup>-1</sup> for L1, L2, L3, L4, L5 and L6, resp., obviously larger than the corresponding value of 0.047 mol<sup>-1</sup> dm<sup>3</sup> s<sup>-1</sup> for the N-methylcyclen-Zn(II)-OH<sup>-</sup> complex catalyst.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 28 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:50616 HCAPLUS Full-text  
 DOCUMENT NUMBER: 133:14149  
 TITLE: Synthesis and biodistribution of R- and S-isomers of  
 [18F]-fluoropropranolol, a lipophilic **ligand**

for the  $\beta$ -adrenergic receptor  
 AUTHOR(S): Tewson, T. J.; Stekhova, S.; Kinsey, B.; **Chen, L.**; Wiens, L.; Barber, R.  
 CORPORATE SOURCE: University of Washington Medical School, Department of Radiology, University of Washington, Seattle, WA, USA  
 SOURCE: Nuclear Medicine and Biology (1999), 26(8), 891-896  
 CODEN: NMBIEO; ISSN: 0969-8051  
 PUBLISHER: Elsevier Science Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The S and R isomers of [18F]-fluoropropriolol (1-[1-fluoro-2-isopropylamino]-3-naphthalen-1-yloxy-propan-2-ol) have been prepared by reductive alkylation of the appropriate aminoalcs. The radiosynthesis provides a reasonable yield (.apprx.25%) to give products of 99% enantiomeric excess and specific activities of 1-3 Ci/ $\mu$ mol. The dissociation consts. for the  $\beta_2$  adrenergic receptor are 0.5 and 2.5 nM for the S and the R isomers, resp. The biodistribution data in rats show that uptake and egress of the tracer is rapid but that the result of blocking studies and the difference between the R and the S isomers suggest receptor-mediated uptake in receptor-rich tissue.  
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 29 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1999:760753 HCAPLUS Full-text  
 DOCUMENT NUMBER: 132:117099  
 TITLE: Efficient discovery of inhibitory **ligands** for diverse targets from a small combinatorial chemical library of chimeric molecules  
 AUTHOR(S): Thorpe, David S.; Edith Chan, A. W.; Binnie, Alan; **Chen, L. Charlie**; Robinson, Anna; Spoonamore, James; Rodwell, David; Wade, Shelly; Wilson, Sydney; Ackerman-Berrier, Martha; Yeoman, Helen; Walle, Stefan; Wu, Qinyuan; Wertman, Kenneth F.  
 CORPORATE SOURCE: Department of Discovery Biology, Selectide Corporation, Tucson, AZ, 85737, USA  
 SOURCE: Biochemical and Biophysical Research Communications (1999), 266(1), 62-65  
 CODEN: BBRC9; ISSN: 0006-291X  
 PUBLISHER: Academic Press  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Living systems are mainly composed and regulated by compds. in four biochem. classes and their polymers-nucleotides, carbohydrates, lipids, and amino acids. Early combinatorial chemical libraries consisted of peptides. The present report describes the general bioactivity and biophys. properties of a combinatorial chemical library that used glyco, nucleotidyl, and lipid building blocks. The resulting chimeric combinatorial library of 361 compds. had a confirmed cumulative hit rate of 0.16%, which is 8-fold higher than a commonly claimed industrial benchmark of 0.02%. It produced 7 structurally confirmed hits for a third of 12 proprietary drug discovery projects, and these comprised a variety of mol. targets. Diversity analyses demonstrated that despite the small number of compds., a wider range of diversity space was covered by this library of biochem. chimeras than by a branched tripeptide library of the same size and similar generic formula. (c) 1999 Academic Press.  
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 30 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:568573 HCAPLUS Full-text

DOCUMENT NUMBER: 131:346079

TITLE: Detection and plasma pharmacokinetics of an anti-vascular endothelial growth factor oligonucleotide-aptamer (NX1838) in rhesus monkeys

AUTHOR(S): Tucker, C. E.; **Chen, L.-S.**; Judkins, M. B.;

Farmer, J. A.; Gill, S. C.; Drolet, D. W.

CORPORATE SOURCE: NeXstar Pharmaceuticals Inc., Boulder, CO, USA

SOURCE: Journal of Chromatography, B: Biomedical Sciences and Applications (1999), 732(1), 203-212  
CODEN: JCBBEP; ISSN: 0378-4347

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Aptamers are oligonucleotide **ligands** selected, in vitro, to bind a specified target protein. The first aptamer to reach human clin. testing is NX1838, a polyethylene glycol conjugated aptamer that inhibits vascular endothelial growth factor. This paper describes the validation of a high-performance liquid chromatog. anion-exchange method for the determination of NX1838 in plasma. Measurements of intact NX1838 had a coefficient of variation of less than 8% and an accuracy between 107% and 115%. The assay was utilized to determine NX1838 plasma pharmacokinetics in rhesus monkeys following a single 1 mg/kg i.v. or s.c. dose. Following i.v. administration, the maximum achieved plasma concentration was 25.5 µg/mL with a terminal half-life of 9.3 h and clearance rate of 6.2 mL/h. After s.c. administration, the fraction of the dose absorbed into the plasma compartment was 0.78 with a time to peak concentration (4.9 µg/mL) of 8 to 12 h.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 31 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:606906 HCAPLUS Full-text

DOCUMENT NUMBER: 129:290094

TITLE: 4-[(1H-Imidazol-4-yl)methyl]benzamidines and benzylamidines: novel antagonists of the histamine H3 receptor

AUTHOR(S): Aslanian, Robert; Brown, Joan E.; **Shih, N.-Y.**

; Mutahi, Mwangi Wa; Green, Michael J.; She, Susan;

Del Prado, Maurice; West, Robert; Hey, John

CORPORATE SOURCE: Schering - Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Bioorganic &amp; Medicinal Chemistry Letters (1998), 8(16), 2263-2268

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:290094

AB A series of amidine substituted phenyl-, benzyl-, and phenethylimidazoles based on the known H3 agonist SK&F 91606 has been synthesized and tested as **ligands** for the histamine H3 receptor. Insertion of a Ph ring between the imidazole ring and the amidine moiety produces antagonists. The benzyl series was found to be the most potent and was further investigated. Some compds. were found to be potent **ligands** for the H3 receptor. In vivo, some compds. were shown to be equipotent to thioperamide, a standard H3 antagonist.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 32 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:432485 HCAPLUS Full-text  
 DOCUMENT NUMBER: 125:135610  
 TITLE: Photochemical crosslinking of type I collagen with hydrophobic and hydrophilic 1,8 naphthalimide dyes  
 AUTHOR(S): Judy, M. M.; **Chen, L.**; Fuh, L.; Nosir, H.; Jackson, R. W.; Matthews, J. L.; Lewis, D. E.; Utecht, R. E.; Yuan, D.  
 CORPORATE SOURCE: Baylor Research Institute, Dallas, TX, USA  
 SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1996), 2681(Laser-Tissue Interaction VII), 53-55  
 CODEN: PSISDG; ISSN: 0277-786X  
 PUBLISHER: SPIE-The International Society for Optical Engineering  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB We have obtained hydrophilic forms of the bifunctional mol. introducing a spacer and **ligands** containing alternating carbon-oxygen bonds (polyethers) wherein the oxygen moieties form hydrogen bonds. Addnl. hydrophilicity is attained by incorporation of an amino group (pos. charge) at the end of each **ligand**. Ongoing studies with these forms of the bifunctional 1,8 naphthalimides have demonstrated welding of meniscal cartilage, articular cartilage, and cornea. These results suggest that the hydrophilic form of the dyes is able to penetrate readily the anionically charged proteoglycan matrix of these tissues and cross-link collagen mols. and possibly the protein cores of the proteoglycans. Gel electrophoretic studies have been performed to assess the photochem. crosslinking of these connective tissue proteins with these new forms of the naphthalimide dyes.

L33 ANSWER 33 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:220484 HCAPLUS Full-text  
 TITLE: Substituted 4 - benzylimidazoles: Novel, potent antagonists of the histamine H3 receptor.  
 AUTHOR(S): Aslanian, Robert; Brown, Joan E.; **Shih, N. -Y.**; Mutahi, Alfred M.; Green, Michael J.; Hey, John; She, Susan; DelPrado, Maurice  
 CORPORATE SOURCE: Schering - Plough Research Institute, Kenilworth, NJ, 07033-0539, USA  
 SOURCE: Book of Abstracts, 211th ACS National Meeting, New Orleans, LA, March 24-28 (1996), MEDI-248. American Chemical Society: Washington, D. C.  
 CODEN: 62PIAJ  
 DOCUMENT TYPE: Conference; Meeting Abstract  
 LANGUAGE: English

AB As part of a program aimed at the discovery of novel H3 **ligands** with potential use in the CNS area, we have synthesized a series of amidine substituted phenyl-, benzyl-, and phenethylimidazoles based on the known H3 agonist SK&F 91606 (I). Insertion of a Ph ring in the Pr chain connecting the imidazole ring and amidine moiety yields compds. that are antagonists. The benzyl series demonstrated the best activity and was further investigated. Compound II was found to be a potent antagonist ( $K_i = 7$  nM) with in vivo activity equivalent to the standard H3 antagonist thioperamide.

L33 ANSWER 34 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:924538 HCAPLUS Full-text  
 TITLE: X-ray absorption studies of model compounds for photosynthesisbischlorophyll cyclophane.  
 AUTHOR(S): **Chen, L. X.**; Wasielewski, M. R.; Svec, W. A.; Huang, K.; Montano, P. A.; Norris, J. R.

CORPORATE SOURCE: Chemistry Division, Argonne National Laboratory,  
Argonne, IL, 60439, USA

SOURCE: Book of Abstracts, 210th ACS National Meeting,  
Chicago, IL, August 20-24 (1995), Issue Pt. 2,  
NUCL-017. American Chemical Society: Washington, D.  
C.

CODEN: 61XGAC

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB The structures of the model compds. for photosynthesis have been determined using X-ray absorption. The common structural features of these model compds. are transition metal substituted chlorophyll dimers with two covalent linkages. Our XAS studies are aimed to determine the ring-ring distance of the dimer in solution using the central metal in the chlorins as probes, and to investigate the solvent effect on coordination state of the dimer. We have found a Zn-Zn distance of about 3.5 Å appearing in the toluene solution of the bis-zinc-chlorophyll cyclophane. This metal-metal interaction diminishes as pyridine is added into the solution. These observation agree with the result of the energy minimized structure of the dimer and the dimer with pyridine as a **ligand** inserted between the dimer. The correlation of the structure and the electron transfer reaction kinetics in similar complexes is studied.

L33 ANSWER 35 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:793024 HCAPLUS Full-text

DOCUMENT NUMBER: 124:8644

TITLE: Preparation of indolyl- and pyrrolylbenzazepines as  
D-1 receptor **ligands**

INVENTOR(S): Berger, Joel G.; Kozlowski, Joseph A.;  
Chang, Wei

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: U.S., 14 pp.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

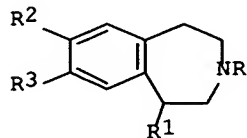
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 5440033	A	19950808	US 1993-149411	19931109
PRIORITY APPLN. INFO.:			US 1993-149411	19931109
OTHER SOURCE(S):	MARPAT	124:8644		

GI



AB Title compds. [I; R = H, alkyl; R1 = (alkyl-substituted) pyrrolyl, indolyl, pyrazolyl; R2 = H, halo, alkyl, CF3; R3 = OH, alkoxy, H2NCO2] were prepared. Thus, 5,8-dichloro-7-methoxy-3-methyl-1H-3-benzazepin-4-one was aminated by 4-iodopyrazole in the presence of KF-Al2O3 (preparation given) and the product treated with LAH to give I (R = Me, R1 = pyrazolo, R2 = Cl, R3 = OMe). I (R =

Me, R1 = 2,5-dimethylpyrrol-3-yl, R2 = Cl, R3 = OH) had minimal ED of 10mg/kg (route of administration not given) for conditioned avoidance response suppression in rats.

L33 ANSWER 36 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:473022 HCAPLUS Full-text

DOCUMENT NUMBER: 123:78257

TITLE: The ternary complex between methylamine dehydrogenase, amicyanin and cytochrome c551i

AUTHOR(S): Mathews, F. S.; **Chen, L.**; Durley, R. C. E.; Davidson, V. L.

CORPORATE SOURCE: Dept. Biochemistry and Molecular Biophysics, Washington University School Medicine, St. Louis, MO, USA

SOURCE: Biochem. Vitam. B6 PQQ, [Int. Meet. Vitam. B6 Carbonyl Catal.] (1994), 291-5. Editor(s): Marino, Gennaro; Sannia, Giovanni; Bossa, Francesco. Birkhaeuser: Basel, Switz. CODEN: 60ZAAX

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The crystal structure of a ternary complex between methylamine dehydrogenase (MADH), amicyanin, and cytochrome c551i, all from *Paracoccus denitrificans*, was determined at 2.4 Å resolution. MADH and amicyanin associated so that the exposed edges of Trp-108 of tryptophan tryptophylquinone (TTQ) and the His-95 **ligand** of Cu were juxtaposed. Amicyanin and cytochrome c551i associated so that one edge of the  $\beta$ -sandwich of amicyanin was in contact with a chain segment of the cytochrome close to the heme propionates. The distance from the catalytically active quinone O atom of TTQ to Cu was 16.8 Å and from Cu to Fe was 24.8 Å, resp. Two efficient paths for electron flow from TTQ to Cu were found, one passing through Trp-108 of MADH. Two paths from Cu to Fe were also found, one through the cysteine and one through the Met **ligand** to Cu, which converged at Tyr-30 of amicyanin.

L33 ANSWER 37 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:266142 HCAPLUS Full-text

DOCUMENT NUMBER: 122:49554

TITLE: Localization and specificity of cytochromes and other electron transfer proteins from sulfate-reducing bacteria

AUTHOR(S): Le Gall, J.; Payne, W. J.; **Chen, L.**; Liu, M. Y.; Xavier, A. V.

CORPORATE SOURCE: Dep. Biochem., Univ. Georgia, Athens, GA, 30602-7220, USA

SOURCE: Biochimie (1994), 76(7), 655-65  
CODEN: BICMBE; ISSN: 0300-9084

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Recently data have accumulated concerning the electron transfer chains of sulfate-reducing bacteria in general and of the genus *Desulfovibrio* in particular. Because of the ever growing number of newly discovered individual redox proteins, it has become essential to try to assign them to physiologically relevant chains. This work presents some new data concerning the localization of these proteins within the bacterial cell and the specificity of electron transfer between the 3 types of hydrogenases which have been found so far in *Desulfovibrio*, namely the Fe-only, the Fe-Ni, and the Fe-Ni-Se enzymes. The Fe-only hydrogenase reduced cytochromes which had bis-histidiny l heme ligation



or histidinyl-methionyl heme ligation. In contrast, the Fe-Ni and Fe-Ni-Se hydrogenases could not reduce cytochromes having a His-Met heme ligation, but were very active toward cytochromes having a bis-histidinyl **ligand**. This observation was used to demonstrate that the tetraheme cytochrome c3 could exchange electrons with the monoheme cytochrome c553. No clear specificity was established for the reaction of hydrogenases toward the hexadecaheme cytochromes from either *D. vulgaris* or *D. gigas*.

L33 ANSWER 38 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:259305 HCAPLUS Full-text  
 DOCUMENT NUMBER: 122:145534  
 TITLE: Charge-transfer transitions of RE<sup>3+</sup>-O<sup>2-</sup> associates in BaF<sub>2</sub> crystal  
 AUTHOR(S): Wang, L. M.; **Chen, L. Y.**; Wu, X.  
 CORPORATE SOURCE: Pohl Inst. Solid State Phys., Tongji Univ., Shanghai, 200092, Peop. Rep. China  
 SOURCE: Materials Research Society Symposium Proceedings (1994), 348(Scintillator and Phosphor Materials), 407-10  
 CODEN: MRSPDH; ISSN: 0272-9172  
 PUBLISHER: Materials Research Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Local-d.-functional calcs. were performed to study the electronic structure and charge-transfer transitions of RE<sup>3+</sup>-O<sup>2-</sup> (RE = Eu and Tm) assocs. in BaF<sub>2</sub> crystal. These systems are simulated by small clusters which are surrounded by over 2000 point charges. The presence of O in the lattice strongly influences the optical properties of RE<sup>3+</sup> ions. The charge transfer transitions of RE<sup>3+</sup>-O<sup>2-</sup> and RE with **ligand** F<sup>-</sup> derived from the embedded cluster are equal to 5.1 and 6.2 eV. The energy gap derived from the HFS model with REOBa<sub>3</sub>F<sub>6</sub> clusters embedded in the crystal is 9.8 eV, which is near the exptl. results.

L33 ANSWER 39 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:63735 HCAPLUS Full-text  
 DOCUMENT NUMBER: 122:155015  
 TITLE: One-electron oxidation of iron(II)-imidazole and iron(II)-bis[imidazol-2-yl]methane complexes: a pulse radiolysis study  
 AUTHOR(S): Parsons, B. J.; Navaratnam, S.; Zhao, Z.; **Chen, L.**  
 CORPORATE SOURCE: Multidisciplinary Research Innovation Centre, North East Wales Institute, Wrexham/Clwyd, LL12 2AW, UK  
 SOURCE: Journal of the Chemical Society, Faraday Transactions (1994), 90(17), 2467-74  
 CODEN: JCFTEV; ISSN: 0956-5000  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The radical anion, Br<sub>2</sub><sup>-</sup>, a strong one-electron oxidant, has been used to oxidize iron(II)-imidazole, FeII-ImH, and iron(II)-bis(imidazol-2-yl)methane, FeII-2-BIM, complexes in aqueous solution, the latter being regarded as good models of the iron(II) site in non-heme iron-containing enzymes such as lipooxygenase. The rates of oxidation of FeII-ImH, FeII(ImH)<sub>2</sub>, Fe-2BIM and FeII(2-BIM)<sub>2</sub> were measured as 1.0+10<sup>7</sup>, 2.0+10<sup>7</sup>, 2.0+10<sup>7</sup>, 1.8+10<sup>8</sup> and 3.6+10<sup>8</sup> dm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup>. From measurements of the rates of oxidation of the **ligand**, it is clear that Br<sub>2</sub><sup>-</sup> oxidizes the **ligand** in the metal complexes in the first instance. The same studies also show that the 2-BIM **ligand** is easier to oxidize than the closely related imidazole **ligand** by a factor of 10.

Measurements of the rate of oxidation of 2-methylimidazole indicate that the difference is attributable to the inductive effect of the -CH<sub>2</sub>- group. The spectra of the transient initial products of the iron(II)-imidazole oxidation are very similar to the imidazole free radical spectra suggesting either very weak metal-ligand charge transfer, MLCT, character in the metal-free radical complex or that the complex dissociates rapidly ( $>10^6$  s<sup>-1</sup>) to yield an imidazole free radical. In contrast, the initial iron(II)-2-BIM products exhibit spectra which are three to six times more intense than the 2-BIM free radical spectrum. For the ML product, this is attributed to MLCT transitions of the metal-2-BIM free radical species, whereas for ML<sub>2</sub>, it is proposed that the spectrum is assigned to an Fe(III)-2-BIM complex, formed following fast intramolecular electron transfer ( $>10^6$  s<sup>-1</sup>) within the Fe(II)-2-BIM free radical complex. The data are in contrast to similar data obtained for iron(II)-histidine complexes in an earlier study (Parsons M. Al-Hakim, G. O. Phillips and A. J. Swallow, J. Chemical Society, Faraday Trans. 1, 1986, 82, 1575) where the oxidation process was not controlled by initial oxidation of the histidine ligand. It is suggested that these differences are attributable to a greater degree of covalent character in the metal ligand bonding in the iron(II)-histidine complex compared with the weaker, largely electrostatic bonds, in iron(II)-imidazole complexes.

L33 ANSWER 40 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:97088 HCAPLUS Full-text

DOCUMENT NUMBER: 120:97088

TITLE: Retroviral gene transfer of epidermal growth factor receptor into HL60 cells results in a partial block of retinoic acid-induced granulocytic differentiation

AUTHOR(S): Chen, Lei L.; Gansbacher, Bernd; Gilboa, Eli; Taetle, Raymond; Oval, John; Hibbs, Margaret S.; Huang, Chi Kuang; Clawson, Michael L.; Bilgrami, Syed  
CORPORATE SOURCE: Health Cent., Univ. Connecticut, Farmington, CT, 06030, USA

SOURCE: Cell Growth & Differentiation (1993), 4(9), 769-76  
CODEN: CGDIE7; ISSN: 1044-9523

DOCUMENT TYPE: Journal

LANGUAGE: English

AB HL60 cells are devoid of endogenous epidermal growth factor receptor (EGFR). They respond to retinoic acid and undergo terminal granulocytic differentiation. EGFR complementary DNA was introduced into HL60 cells by retroviral gene transfer. Scatchard plot showed that the binding characteristics are identical to those of A431 cells. HL60-EGFR cells were estimated to express 34,000 EGFR/cell ( $K_d = 5$  nM). The tyrosine phosphorylation upon ligand binding is the first step of signal transduction. The dominant phosphotyrosyl proteins in epidermal growth factor-stimulated HL60-EGFR cells include a 170 kDa protein (EGFR itself), and 125 and 53 kDa proteins. The EGFR signal results in the induction of 92 kDa gelatinase/matrix metalloproteinase in HL60-EGFR cells, thereby providing evidence of the function of the exogenous EGFR and a semiquantitative measure of the EGFR signal. These HL60-EGFR cells offer a unique opportunity to examine the potentially important role of EGFR (c-erbB) in maintaining homeostasis between self-renewal and differentiation. The c-erbB has been shown to play a physiological role in the self-renewal of the very early avian stem cells which do express EGFR. The v-erbB (double truncated EGFR) has been shown to cause avian erythroblastosis. The authors found that these HL60-EGFR cells responded to retinoic acid differently from the HL60-control cells. A partial block of only 45% granulocytic differentiation and concomitant proliferation was noted, consistent with a shift of balance between self-renewal and differentiation toward the former.

L33 ANSWER 41 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:40323 HCAPLUS Full-text

DOCUMENT NUMBER: 120:40323

TITLE: Electrochemistry of platinum phosphine complexes: carbon-hydrogen and carbon-halide activation by highly reactive intermediates

AUTHOR(S): Davies, J. A.; Chen, L.; Eagle, C. T.; Staples, R. J.

CORPORATE SOURCE: Dep. Chem., Univ. Toledo, Toledo, OH, 43606, USA

SOURCE: NATO ASI Series, Series C: Mathematical and Physical Sciences (1993), 385 (Molecular Electrochemistry of Inorganic, Bioinorganic and Organometallic Compounds), 351-6

CODEN: NSCSDW; ISSN: 0258-2023

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 18 refs. is given. The electrochem. reduction of cis-[PtX<sub>2</sub>L<sub>2</sub>] (X = halide, L = tertiary phosphine) complexes in CH<sub>3</sub>CN/C<sub>6</sub>H<sub>6</sub>/TBAP (Hg electrode) generates [PtL<sub>2</sub>] equivalent. The reactivity of these complexes is determined by the nature of the monodentate phosphine ligands, e.g. when L = PPh<sub>3</sub> the complex does not react with benzonitrile but when L = PEt<sub>3</sub> the complex reacts with PhCN via oxidative addition of the rather inert C-CN bond. When the monodentate ligands are replaced by a bidentate ligand, electrochem. reduction leads to the generation of nonlinear [Pt(bidentate)] complexes. The reactivity is altered by the presence of the bidentate ligand, e.g. when L<sub>2</sub> = (c-Hx)<sub>2</sub>P(CH<sub>2</sub>)<sub>3</sub>P(c-Hx)<sub>2</sub>, generation of [Pt(bidentate)] in CH<sub>3</sub>CN/C<sub>6</sub>H<sub>6</sub>/TBAP results in C-H oxidative addition of benzene to produce a phenylplatinum(II) hydride complex. This contrasts with the electrochem. generation of [Pt(PEt<sub>3</sub>)<sub>2</sub>] in the same medium where a subsequent acid/base reaction with the N(n-Bu)<sub>4</sub><sup>+</sup> cation leads to the formation of trans-[PtH(Cl)(PEt<sub>3</sub>)<sub>2</sub>] with production of tri(n-butyl)amine. Electrochem. reduction of trans-[PtH(Cl)(PEt<sub>3</sub>)<sub>2</sub>] in CH<sub>3</sub>CN/C<sub>6</sub>H<sub>6</sub>/TBAP (Hg electrode) results in H- transfer to CH<sub>3</sub>CN and then further reactions due to the cyanomethyl anion that is produced. Electrochem. oxidation of trans-[PtH(Cl)(PEt<sub>3</sub>)<sub>2</sub>] at a platinum mesh electrode does not lead to transformation of Pt(II) into Pt(IV) but rather induces the formal oxidation of H- to H<sup>+</sup>. Reduction of the platinum(II) aryl complex [PtPh<sub>2</sub>L<sub>2</sub>] (L<sub>2</sub> = Ph<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PPh<sub>2</sub>) in CH<sub>3</sub>CN/TBAP (Hg electrode) leads to cleavage of the Pt-C bonds and formation of benzene (but not biphenyl) through scavenging of the organic fragments. Cleavage of Pt-C bonds can similarly be induced by oxidation in certain cases and this process is the main focus of the current report. Thus, although oxidative electrolysis of cis-[PtPh<sub>2</sub>(PEt<sub>3</sub>)<sub>2</sub>] in CH<sub>3</sub>CN produces the expected [PtPh<sub>2</sub>(CH<sub>3</sub>CN)<sub>2</sub>(PEt<sub>3</sub>)<sub>2</sub>]<sup>2+</sup> without Pt-C bond cleavage, oxidation of the benzylplatinum(II) complexes trans-[PtBz(Cl)(PEt<sub>3</sub>)<sub>2</sub>] and cis-[PtBz<sub>2</sub>(PEt<sub>3</sub>)<sub>2</sub>] generates benzyl alc. and benzaldehyde via oxidation of the cleaved organic fragments. These results demonstrate not only that C-H and C-X bond cleavage, accompanied by Pt-H, Pt-X, and Pt-C bond formation, can be induced by electrochem. strategies but also that Pt-H and Pt-C cleavage processes, accompanied by the formation of useful organic products, can be achieved with the use of electrochem. methods.

L33 ANSWER 42 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:671158 HCAPLUS Full-text

DOCUMENT NUMBER: 119:271158

TITLE: (Amidazolylakyl)piperidines which are histamine H<sub>3</sub> receptor antagonists or agonists

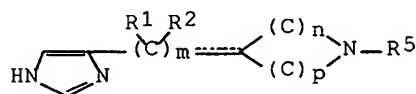
INVENTOR(S): Shih, Neng Yang; Green, Michael J.

PATENT ASSIGNEE(S): Schering Corp., USA

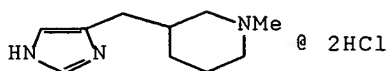
SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9312107	A1	19930624	WO 1992-US10698	19921216
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KR, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9332758	A1	19930719	AU 1993-32758	19921216
AU 665604	B2	19960111		
EP 619818	A1	19941019	EP 1993-901399	19921216
EP 619818	B1	19960710		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 06511252	T2	19941215	JP 1992-511084	19921216
JP 07121938	B4	19951225		
AT 140223	E	19960715	AT 1993-901399	19921216
ES 2089782	T3	19961001	ES 1993-901399	19921216
CA 2126086	C	20000328	CA 1992-2126086	19921216
ZA 9209785	A	19930621	ZA 1992-9785	19921217
IL 104124	A1	19981206	IL 1992-104124	19921217
US 5807872	A	19980915	US 1994-244830	19940615
PRIORITY APPLN. INFO.:			US 1991-810651	A2 19911218
			WO 1992-US10698	A 19921216
OTHER SOURCE(S):		MARPAT 119:271158		
GI				



I



II

AB The title compds. I [R1-R4 = H, C1-6 alkyl, (CH2)qR6, OR7, CO2R7, COR7, O2CR7, CONR7R8, CN, SR7, etc.; R6 = (un)substituted Ph; R7, R8 = OH, C1-6 alkoxy, halogen, C1-6 alkyl, CF3, CN, NO2, etc.; q = 1-7; R5 = H, C1-20 alkyl, C3-6 cycloalkyl, CO2R7, COR7, CONR7R8, allyl, propargyl, (CH2)qR6; m = 1,2; n, p = 0-4; such that n + p = 4; the dotted line represents a double bond that is optionally present when m = 1 and n ≠ 0, when the double bond is present R2 is absent], which are antagonists or agonists of histamine H3 receptors and useful in treatment of central nervous system disorders (no data), are prepared. Thus, N-methyl-2-piperidinone was reacted with LiN(Pr-iso)2, the intermediate condensed with 4-(chloromethyl)-N-tritylimidazole, the condensate reacted with LiAlH4, and the reaction mixture treated with HCl solution, producing imidazole derivative II. II demonstrated an inhibition of radioactive ligand binding to histamine H3 receptor isolated from guinea pig brain.

L33 ANSWER 43 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1990:418303 HCAPLUS Full-text  
 DOCUMENT NUMBER: 113:18303  
 TITLE: Characterization and tissue distribution of H3

histamine receptors in guinea pigs by  
 $\alpha$ -methylhistamine  
 AUTHOR(S): Korte, Alexandra; Myers, Joyce; **Shih, Neng Yang**; Egan, Robert W.; Clark, Mike A.  
 CORPORATE SOURCE: Dep. Allergy Immunol., Schering-Plough Res.,  
 Bloomfield, NJ, 07003, USA  
 SOURCE: Biochemical and Biophysical Research Communications  
 (1990), 168(3), 979-86  
 CODEN: BBRC9; ISSN: 0006-291X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB [3H] $\alpha$ -methylhistamine was used to characterize H3-receptor binding in the guinea pig brain and to study its tissue distribution. Kinetic and equilibrium binding expts. indicate a single class of high-affinity sites in membranes isolated from guinea pig brain tissue (dissociation constant = 0.4 nM, receptor d. = 41 fmol/kg protein). Competition binding expts. have confirmed that this **ligand** assoc. with H3-receptors and, under the conditions used in these expts., does not bind to H1- or H2-receptors. Although there was some binding in the ileum and large intestine, H3-binding was found primarily in the central nervous system.

L33 ANSWER 44 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:153700 HCAPLUS Full-text  
 DOCUMENT NUMBER: 110:153700  
 TITLE: Dynamics of molecular recognition involving  
 cucurbituril  
 AUTHOR(S): Mock, William L.; **Shih, Neng Yang**  
 CORPORATE SOURCE: Dep. Chem., Univ. Illinois, Chicago, IL, 60680, USA  
 SOURCE: Journal of the American Chemical Society (1989),  
 111(7), 2697-9  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB For the synthetic receptor cucurbituril, the rate of inclusion complex formation correlates with mol. diameter of alkylammonium ion **ligands**, but not with the thermodyn. stability of the complexes formed. Measurements of <sup>13</sup>C NMR spin-lattice relaxation allow comparison of mol. tumbling motions of the receptor with those of bound **ligands**, by determination at their resp. correlation times. Guest ions appear to rotate relatively freely within cucurbituril, irres. of the stability of the complexes. Results are interpreted in terms of shape complementarity between receptor and **ligand**.

L33 ANSWER 45 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:437470 HCAPLUS Full-text  
 DOCUMENT NUMBER: 109:37470  
 TITLE: Organic **ligand**-receptor interactions between  
 cucurbituril and alkylammonium ions  
 AUTHOR(S): Mock, William L.; **Shih, Neng Yang**  
 CORPORATE SOURCE: Dep. Chem., Univ. Illinois, Chicago, IL, 60680, USA  
 SOURCE: Journal of the American Chemical Society (1988),  
 110(14), 4706-10  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Exptl. binding energies for 24 substituted ammonium ion **ligands** for the synthetic receptor curcurbituril (I) are adjusted for **ligand** solvation and then factored by regression anal. into contributions from various fragments of the **ligands** in their inclusion complexes. This allows quant. estimation of

noncovalent forces occurring in the interaction of **ligand** with receptor. The center of I constitutes a lipophilic region, but the entrances to the interior (ammonium ion binding site) are countervailingly lipophobic. Enhanced dispersion forces involving the sulfide functional group may exist in the receptor complexes of such **ligands**, but they make no extra contribution to the hydrophobic effect generally. The specificity of I as a mol. receptor is explained in terms of ion-dipole attractions and shape complementarity with **ligands**.

L33 ANSWER 46 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:591296 HCAPLUS Full-text  
 DOCUMENT NUMBER: 105:191296  
 TITLE: **Ligand** mixing in lower order organocuprates:  
 synthetic, mechanistic, and structural implications  
 AUTHOR(S): Lipshutz, Bruce H.; Kozlowski, Joseph A.;  
 Breneman, Curt M.  
 CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA,  
 93106, USA  
 SOURCE: Tetrahedron Letters (1985), 26(48), 5911-14  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB NMR spectroscopic evidence attesting to facile **ligand** exchange between lower order cuprates in THF and Et<sub>2</sub>O solution is discussed. A mechanistic pathway is suggested to account for **ligand** redistribution in THF. A dimeric model for R<sub>2</sub>CuLi is supported by the spectral data.

L33 ANSWER 47 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:453344 HCAPLUS Full-text  
 DOCUMENT NUMBER: 103:53344  
 TITLE: More highly mixed, higher order cyanocuprates  
 "RT(2-thienyl)Cu(CN)Li<sub>2</sub>". Efficient reagents which  
 promote selective **ligand** transfer  
 AUTHOR(S): Lipshutz, Bruce H.; Kozlowski, Joseph A.;  
 Parker, David A.; Nguyen, Sam L.; McCarthy, Keith E.  
 CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA,  
 93106, USA  
 SOURCE: Journal of Organometallic Chemistry (1985), 285(1-3),  
 437-47  
 CODEN: JORCAI; ISSN: 0022-328X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 103:53344

AB The combination of RLi (R = vinyl, Pr, Bu, CHMeEt, CMe<sub>3</sub>, Ph) and 2-lithiothiophene with CuCN forms the title reagent. This species selectively transfers the R **ligand** in substitution reactions with epoxides and halides. With unhindered substrates, the cuprate reacts in conjugate addition processes, whereas  $\beta,\beta$ -disubstituted compds. unexpectedly afford products resulting from 1,2-addition of the thiophene group. The prospects for use of these reagents in the synthesis of polyene macrolide antibiotics are discussed.

L33 ANSWER 48 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:570341 HCAPLUS Full-text  
 DOCUMENT NUMBER: 101:170341  
 TITLE: Conjugate addition reactions of  $\alpha,\beta$ -unsaturated ketones with higher order, mixed

organocuprate reagents,  $\text{R}_2\text{Cu}(\text{CN})\text{Li}_2$   
 AUTHOR(S): Lipshutz, Bruce H.; Wilhelm, Robert S.;  
**Kozlowski, Joseph A.**  
 CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA,  
 93106, USA  
 SOURCE: Journal of Organic Chemistry (1984), 49(21), 3938-42  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 101:170341

AB Conjugate addition reactions of  $\text{R}_2\text{Cu}(\text{CN})\text{Li}_2$  (I) with  $\alpha,\beta$ -unsatd. ketones are reported. These reagents, in most cases, react extremely rapidly to give the corresponding alkylated ketones in high yields. Attempts at trapping the intermediate enolates were successful using MeI as electrophile; however, the method is not general and was therefore not pursued. The effects of solvent and **ligand** composition on I, as well as on the more highly mixed species  $\text{RR}_1\text{Cu}(\text{CN})\text{Li}_2$ , were examined. The selectivity of **ligand** transfer in these latter, 2nd-generation organocuprates is also discussed.

L33 ANSWER 49 OF 50 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:570200 HCAPLUS Full-text  
 DOCUMENT NUMBER: 101:170200  
 TITLE: Substitution reactions of secondary halides and  
 epoxides with higher order, mixed organocuprates,  
 $\text{R}_2\text{Cu}(\text{CN})\text{Li}_2$ : synthetic, stereochemical, and  
 mechanistic aspects  
 AUTHOR(S): Lipshutz, Bruce H.; Wilhelm, Robert S.;  
**Kozlowski, Joseph A.**; Parker, David  
 CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA,  
 93106, USA  
 SOURCE: Journal of Organic Chemistry (1984), 49(21), 3928-38  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 101:170200

AB  $\text{R}_2\text{Cu}(\text{CN})\text{Li}_2$  (R = alkyl, alkenyl, aryl) are readily prepared from CuCN and 2 equivalent of an organolithium. These novel reagents react readily and efficiently with secondary unactivated iodides and bromides affording products of substitution. Likewise, mono-, di-, and trisubstituted epoxides undergo ring opening leading to the corresponding alcs. in excellent yields. The effects of solvent, temperature, gegenion, and variations in **ligands** are discussed. In mixed **ligand** cuprates  $\text{R}(\text{CH}_3)\text{Cu}(\text{CN})\text{Li}_2$ , the R group is preferentially transferred in reactions with halides.

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 TITLE: Chemistry of higher order, mixed organocuprates. 5.  
 On the choice of the copper(I) salt for the formation  
 of  $\text{R}_2\text{CuLi}$   
 AUTHOR(S): Lipshutz, Bruce H.; **Kozlowski, Joseph A.**;  
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 SOURCE: Journal of Organic Chemistry (1983), 48(4), 546-50  
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AB Chemical and spectroscopic studies are presented that have been designed to manifest differences in reagent composition and reactivity between mixts. of CuI/2RLi and CuSCN/2RLi (R = Me, Pr, Bu, Ph). The results indicate that while both Cu(I) salts are reported to serve as precursors to lower order cuprates R<sub>2</sub>CuLi, CuSCN may actually be forming a higher order, mixed species R<sub>2</sub>Cu(SCN)Li<sub>2</sub>. This would explain the discrepancy in coupling reactions of each solution with similar organic substrates under otherwise identical conditions. The presence of added lithium salts demonstrates that while LiI added to CuSCN/2RLi has essentially no effect, introduction of an equivalent of LiSCN to CuI/2RLi dramatically alters the efficiency of **ligand** transfer.